



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1OLZ
Title : THE LIGAND-BINDING FACE OF THE SEMAPHORINS REVEALED BY
THE HIGH RESOLUTION CRYSTAL STRUCTURE OF SEMA4D
Authors : Love, C.A.; Harlos, K.; Mavaddat, N.; Davis, S.J.; Stuart, D.I.; Jones, E.Y.;
Esnouf, R.M.
Deposited on : 2003-08-19
Resolution : 2.00 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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

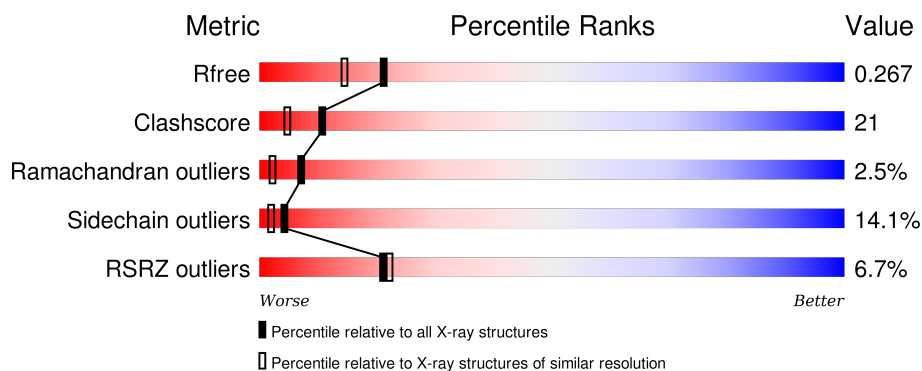
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	663	 5% 57% 28% 8% • 6%
1	B	663	 7% 60% 26% 8% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10669 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 SEMAPHORIN 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			
1	B	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	398	Total	O	0	0
			398	398		
2	B	443	Total	O	0	0
			443	443		

LEU	L573	R464	R345	V224
SER	K574	N471	F346	F225
VAL	A575	S472	D351	R226
VAL	E576	G473	S352	I229
GLN	S577	V474	E353	P230
THR	P578	V475	A354	R231
GLU	K579		R355	
GLY	T580	L479	A356	R234
SER	G581		A357	
ARG	L582	K484	N358	Q240
ILE	M583			
ALA	G584	E489	T369	R257
THR	R585		L370	
LYS	K586	R495	Q371	R262
VAL	N587	P503	F372	P263
LEU	L588	P504	D380	D264
VAL	L589			S265
VAL	I590			
ALA	I591	L511	I386	L272
SER	F591	H512	D387	
THR	N592	Q513	N388	L278
LYS	L593		R389	R279
HIS	S594	M525	P390	S280
HIS	E595	S526	R391	P281
HIS	G596	G527	L392	G282
HIS	D597	C532	I393	L283
HIS	S598	P533	K394	K284
HIS	S599	D534	K395	V285
HIS	G599	K335	D396	
	Y601	S336	V397	L291
		R337	N398	N297
		G538	Y399	
			V403	L301
		R541	Q408	N308
		Q542	V409	L309
		H543	L410	
		F544		K320
		F545	V414	Y321
				M322
		T550	M418	Q323
		A551	F419	S324
		E552		T325
			E434	T326
		C555	H435	V327
		S556		E328
		Q557		Q329
			F446	S330
		A562	Q447	H331
		R563	D448	
		V564		T332
			Q453	K333
		F565		W334
		W566	S458	V335
		PRQ	K567	R336
		PRQ	F568	
		VAL	S459	
		VAL	K460	
		VAL	R461	
		ALA	G462	P342
		PRQ	G571	K343
		THR	V572	P344

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.32Å 76.76Å 89.41Å 77.41° 73.35° 63.57°	Depositor
Resolution (Å)	20.00 – 2.00 19.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.00) 93.6 (19.51-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.270 0.206 , 0.267	Depositor DCC
R_{free} test set	5440 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 107916 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10669	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/5034	0.64	1/6825 (0.0%)
1	B	0.39	0/5034	0.68	2/6825 (0.0%)
All	All	0.39	0/10068	0.66	3/13650 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	SER	C-N-CD	-7.49	104.11	120.60
1	B	199	SER	C-N-CA	6.12	147.71	122.00
1	A	457	LEU	CA-CB-CG	5.20	127.25	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	4914	0	4841	223	0
1	B	4914	0	4841	198	0
2	A	398	0	0	24	0
2	B	443	0	0	39	0
All	All	10669	0	9682	414	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 21.

All (414) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:HG3	1:A:495:ARG:HH11	1.06	1.12
1:A:608:ARG:HD2	1:A:608:ARG:H	1.13	1.12
1:B:200:PRO:HD3	1:B:205:GLY:HA2	1.35	1.08
1:B:343:LYS:HB3	1:B:344:PRO:HD3	1.33	1.07
1:B:199:SER:HB3	1:B:200:PRO:C	1.82	1.00
1:B:543:HIS:HB2	1:B:623:LEU:HB2	1.43	0.96
1:A:609:VAL:HG22	1:A:610:LYS:H	1.31	0.96
1:A:527:GLY:HA3	1:A:609:VAL:HG21	1.50	0.94
1:A:323:GLN:HE21	1:A:325:THR:HG22	1.32	0.93
1:A:200:PRO:HD2	1:A:206:GLU:HB2	1.51	0.92
1:A:557:GLN:HE22	1:A:562:ALA:HB3	1.35	0.91
1:A:608:ARG:CD	1:A:608:ARG:H	1.81	0.91
1:B:460:LYS:HA	1:B:464:ARG:HE	1.36	0.91
1:B:600:VAL:HG22	1:B:622:VAL:HG22	1.51	0.90
1:B:343:LYS:HB3	1:B:344:PRO:CD	2.01	0.89
1:A:495:ARG:HG3	1:A:495:ARG:NH1	1.84	0.89
1:B:410:LEU:HD13	1:B:511:LEU:HD11	1.56	0.88
1:A:608:ARG:HD2	1:A:608:ARG:N	1.88	0.87
1:A:197:ARG:HG3	1:A:198:LYS:H	1.39	0.86
1:B:94:LEU:HD22	2:B:2042:HOH:O	1.74	0.86
1:A:200:PRO:HD2	1:A:206:GLU:CB	2.07	0.82
1:A:36:GLU:OE2	1:A:99:ALA:HA	1.78	0.82
1:A:609:VAL:HG22	1:A:610:LYS:N	1.95	0.81
1:A:280:SER:OG	1:A:283:LEU:HB2	1.81	0.81
1:A:283:LEU:HG	1:A:406:ARG:HH12	1.47	0.79
1:A:330:SER:HB2	2:A:2254:HOH:O	1.83	0.77
1:B:545:PHE:O	1:B:625:VAL:HA	1.84	0.77
1:A:557:GLN:NE2	1:A:562:ALA:HB3	1.99	0.77
1:A:584:GLY:O	1:A:586:LYS:HG2	1.84	0.77
1:A:343:LYS:HB3	1:A:344:PRO:HD3	1.66	0.77
1:B:12:GLU:HB2	1:B:15:GLU:HG2	1.67	0.76
1:A:320:LYS:HE3	1:A:336:ARG:HD3	1.69	0.74
1:A:325:THR:O	1:A:326:THR:HG22	1.86	0.74
1:B:495:ARG:NH1	1:B:609:VAL:HG23	2.01	0.74
1:B:343:LYS:CB	1:B:344:PRO:HD3	2.14	0.73
1:B:543:HIS:HB2	1:B:623:LEU:CB	2.19	0.73
1:A:504:PRO:CG	1:A:517:PRO:HG3	2.18	0.73
1:B:199:SER:HB3	1:B:200:PRO:O	1.89	0.72
1:B:537:LYS:HD3	1:B:617:VAL:O	1.88	0.72
1:A:265:SER:HB3	1:A:267:LEU:HG	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:O	1:A:435:HIS:HB2	1.89	0.71
1:B:460:LYS:CA	1:B:464:ARG:HE	2.04	0.70
1:B:44:GLY:HA3	2:B:2042:HOH:O	1.90	0.70
1:A:552:GLU:O	1:A:552:GLU:HG3	1.92	0.70
1:B:543:HIS:CB	1:B:623:LEU:HB2	2.19	0.69
1:A:549:GLY:O	1:A:593:LEU:HB2	1.93	0.69
1:B:513:GLN:HG3	2:B:2398:HOH:O	1.93	0.69
1:A:608:ARG:HH11	1:A:608:ARG:HG3	1.56	0.68
1:B:408:GLN:HG3	1:B:414:VAL:HG22	1.76	0.68
1:B:527:GLY:HA3	1:B:609:VAL:HG21	1.75	0.68
1:B:537:LYS:NZ	1:B:617:VAL:H	1.91	0.68
1:A:134:ARG:NH2	1:A:170:ASN:HB3	2.08	0.68
1:B:557:GLN:HB2	2:B:2431:HOH:O	1.92	0.68
1:A:326:THR:O	1:A:332:THR:HA	1.94	0.68
1:A:541:ARG:HG2	1:A:543:HIS:NE2	2.08	0.68
1:B:610:LYS:HB2	2:B:2439:HOH:O	1.93	0.67
1:A:323:GLN:NE2	1:A:325:THR:HG22	2.08	0.67
1:A:283:LEU:HG	1:A:406:ARG:NH1	2.08	0.67
1:A:533:PRO:HG2	2:A:2363:HOH:O	1.95	0.66
1:B:585:ARG:O	1:B:586:LYS:HB2	1.93	0.66
1:A:330:SER:HB3	2:A:2256:HOH:O	1.94	0.66
1:B:545:PHE:HD2	1:B:623:LEU:HD12	1.61	0.66
1:A:504:PRO:HG3	1:A:517:PRO:HG3	1.77	0.66
1:A:594:SER:O	1:A:625:VAL:HG11	1.96	0.66
1:B:573:LEU:HD23	1:B:573:LEU:C	2.16	0.65
1:B:262:ARG:HG2	1:B:264:ASP:OD1	1.97	0.65
1:A:333:LYS:NZ	1:B:333:LYS:HB2	2.12	0.65
1:B:447:GLN:HG3	2:B:2012:HOH:O	1.97	0.65
1:A:545:PHE:CD2	1:A:623:LEU:HD11	2.31	0.65
1:B:35:SER:HB3	1:B:38:LYS:O	1.96	0.65
1:B:535:LYS:O	1:B:537:LYS:N	2.28	0.65
1:B:200:PRO:HD3	1:B:205:GLY:CA	2.22	0.64
1:A:516:SER:HB3	1:A:517:PRO:HD2	1.79	0.64
1:A:512:HIS:O	1:A:513:GLN:HB3	1.97	0.64
1:A:557:GLN:HG2	1:A:558:LYS:N	2.13	0.63
1:B:333:LYS:HE2	1:B:335:VAL:HG12	1.80	0.63
1:B:458:SER:O	1:B:464:ARG:NH2	2.31	0.63
1:A:576:GLU:CD	1:A:577:SER:H	2.01	0.63
1:A:12:GLU:HG2	1:A:15:GLU:OE1	1.98	0.63
1:A:200:PRO:CD	1:A:206:GLU:HB2	2.27	0.62
1:B:75:LYS:HE3	1:B:111:GLN:OE1	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLU:HB2	2:B:2159:HOH:O	1.99	0.62
1:B:125:LEU:HD12	1:B:127:LYS:HE2	1.80	0.62
1:B:537:LYS:HZ3	1:B:617:VAL:H	1.47	0.62
1:A:148:VAL:HG22	1:A:195:VAL:CG1	2.30	0.62
1:A:28:ASN:HD22	1:A:471:ASN:ND2	1.97	0.62
1:B:542:GLN:H	1:B:542:GLN:CD	2.03	0.61
1:A:586:LYS:HE3	2:A:2390:HOH:O	2.00	0.61
1:B:585:ARG:O	1:B:586:LYS:CB	2.47	0.61
1:A:541:ARG:HG2	1:A:543:HIS:CE1	2.34	0.61
1:B:527:GLY:HA3	1:B:609:VAL:CG2	2.31	0.61
1:B:326:THR:O	1:B:326:THR:HG23	2.00	0.61
1:A:582:LEU:HD23	1:A:585:ARG:HA	1.83	0.60
1:A:582:LEU:HA	1:A:587:ASN:O	2.01	0.60
1:B:566:TRP:HB2	1:B:573:LEU:HD22	1.83	0.60
1:B:12:GLU:HG2	1:B:15:GLU:OE2	2.01	0.60
1:A:528:ASP:OD1	1:A:612:LYS:HD3	2.01	0.60
1:B:464:ARG:HD3	2:B:2329:HOH:O	2.01	0.60
1:B:73:LYS:HG2	1:B:83:LYS:HD3	1.83	0.60
1:B:38:LYS:H	1:B:38:LYS:HE2	1.66	0.60
1:B:551:ALA:HB3	2:B:2424:HOH:O	2.01	0.60
1:B:351:ASP:HB2	2:B:2281:HOH:O	2.01	0.59
1:B:503:PRO:N	1:B:504:PRO:HD2	2.17	0.59
1:B:535:LYS:O	1:B:537:LYS:HE3	2.01	0.59
1:A:30:SER:HB3	2:A:2322:HOH:O	2.01	0.59
1:A:391:ARG:HH11	1:A:391:ARG:CG	2.16	0.59
1:A:545:PHE:HD2	1:A:623:LEU:HD11	1.67	0.59
1:A:148:VAL:HG22	1:A:195:VAL:HG11	1.84	0.59
1:A:541:ARG:HB2	1:A:541:ARG:CZ	2.32	0.59
1:B:495:ARG:HH11	1:B:609:VAL:HG23	1.65	0.59
1:A:460:LYS:HD2	2:A:2336:HOH:O	2.02	0.59
1:B:279:ARG:O	1:B:280:SER:O	2.21	0.59
1:B:343:LYS:CB	1:B:344:PRO:CD	2.78	0.59
1:A:197:ARG:HG3	1:A:198:LYS:N	2.15	0.58
1:B:590:ILE:HB	2:B:2424:HOH:O	2.02	0.58
1:A:343:LYS:HZ2	1:A:343:LYS:HA	1.68	0.58
1:A:386:ILE:O	1:A:387:ASP:HB2	2.02	0.58
1:A:327:VAL:O	1:A:327:VAL:HG13	2.02	0.58
1:A:516:SER:HB3	1:A:521:LEU:HD21	1.86	0.57
1:A:333:LYS:HZ2	1:B:333:LYS:HB2	1.69	0.57
1:B:36:GLU:HA	2:B:2034:HOH:O	2.05	0.57
1:B:573:LEU:HA	1:B:574:LYS:HE3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LYS:HE2	1:B:63:GLU:OE2	2.04	0.57
1:A:495:ARG:HH11	1:A:495:ARG:CG	1.96	0.57
1:A:281:PRO:HD2	2:A:2234:HOH:O	2.05	0.57
1:A:56:ASN:ND2	2:A:2072:HOH:O	2.37	0.57
1:B:240:GLN:HG2	2:B:2152:HOH:O	2.05	0.57
1:B:460:LYS:HA	1:B:464:ARG:NE	2.16	0.57
1:B:574:LYS:O	1:B:576:GLU:N	2.38	0.57
1:A:330:SER:O	1:A:331:HIS:HB2	2.06	0.56
1:A:434:GLU:O	1:A:435:HIS:CB	2.53	0.56
1:B:489:GLU:OE1	1:B:537:LYS:HE2	2.05	0.56
1:B:418:MET:HE2	2:B:2343:HOH:O	2.04	0.56
1:A:179:GLU:OE1	1:A:374:LYS:HE3	2.05	0.56
1:A:211:TYR:CE1	1:A:234:ARG:HG2	2.40	0.56
1:A:343:LYS:HB3	1:A:344:PRO:CD	2.34	0.56
1:A:394:LYS:HG2	1:A:397:VAL:HG11	1.88	0.56
1:A:71:ASP:O	1:A:74:ALA:HB3	2.06	0.56
1:B:31:ALA:HB3	2:B:2042:HOH:O	2.06	0.55
1:B:131:GLY:HA2	1:B:134:ARG:HD2	1.88	0.55
1:A:563:ARG:HB3	1:A:606:GLU:OE2	2.06	0.55
1:B:344:PRO:HD2	1:B:369:THR:OG1	2.06	0.55
1:A:3:PHE:CD1	1:A:395:LYS:HG3	2.41	0.55
1:B:229:ILE:HG12	1:B:257:ARG:HG2	1.88	0.55
1:B:200:PRO:CD	1:B:205:GLY:HA2	2.24	0.55
1:B:595:GLU:OE1	1:B:625:VAL:HG13	2.06	0.55
1:B:463:ASN:ND2	1:B:513:GLN:NE2	2.54	0.55
1:A:78:GLU:HA	2:A:2109:HOH:O	2.06	0.55
1:A:97:LEU:HG	1:A:103:TYR:HB2	1.89	0.55
1:A:545:PHE:O	1:A:626:LYS:HG3	2.07	0.55
1:B:327:VAL:HG22	1:B:328:GLU:OE2	2.05	0.55
1:A:81:LYS:HD2	1:A:110:PHE:CZ	2.42	0.55
1:B:392:LEU:C	1:B:392:LEU:HD23	2.27	0.55
1:B:121:SER:OG	1:B:123:LYS:HB2	2.07	0.55
1:A:326:THR:HG23	1:A:331:HIS:O	2.07	0.54
1:A:151:GLU:CD	1:A:171:SER:HB3	2.28	0.54
1:B:545:PHE:HB3	1:B:593:LEU:HD12	1.89	0.54
1:A:510:ALA:O	1:A:514:THR:HB	2.07	0.54
1:B:453:GLN:HE22	1:B:471:ASN:ND2	2.06	0.54
1:B:594:SER:OG	1:B:595:GLU:N	2.40	0.54
1:A:359:TYR:HA	1:A:364:ASN:OD1	2.07	0.54
1:A:151:GLU:HG3	2:A:2177:HOH:O	2.08	0.54
1:B:550:THR:HG23	2:B:2423:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ARG:HD2	1:A:338:ASN:HD21	1.71	0.54
1:B:386:ILE:O	1:B:387:ASP:HB2	2.08	0.54
1:A:516:SER:CB	1:A:521:LEU:HD21	2.38	0.53
1:B:222:GLU:HA	1:B:222:GLU:OE1	2.07	0.53
1:B:545:PHE:O	1:B:625:VAL:CA	2.54	0.53
1:B:568:PHE:O	1:B:569:GLN:C	2.47	0.53
1:B:418:MET:CE	2:B:2343:HOH:O	2.56	0.53
1:B:544:PHE:HB3	1:B:626:LYS:NZ	2.24	0.53
1:B:97:LEU:HG	1:B:103:TYR:HB2	1.89	0.53
1:A:556:SER:HB2	1:A:586:LYS:HD2	1.91	0.53
1:B:604:LEU:HD23	1:B:604:LEU:N	2.24	0.53
1:A:606:GLU:HB3	1:A:615:PHE:CE1	2.44	0.53
1:A:242:GLY:HA3	1:A:245:THR:O	2.08	0.53
1:B:59:GLU:HG3	2:B:2046:HOH:O	2.08	0.53
1:A:512:HIS:O	1:A:513:GLN:CB	2.56	0.53
1:A:93:VAL:HB	1:A:105:CYS:HB2	1.91	0.52
1:A:511:LEU:O	1:A:512:HIS:C	2.47	0.52
1:A:577:SER:OG	1:A:578:PRO:HA	2.09	0.52
1:B:118:ASN:O	1:B:122:PHE:N	2.42	0.52
1:A:69:SER:OG	1:A:72:LYS:HB2	2.09	0.52
1:B:460:LYS:N	1:B:464:ARG:HH21	2.07	0.52
1:A:5:PRO:HG2	2:A:2005:HOH:O	2.08	0.52
1:A:130:ASP:OD2	1:A:132:LYS:HB2	2.10	0.52
1:A:586:LYS:HG3	1:A:587:ASN:N	2.25	0.52
1:A:547:HIS:HB2	1:A:626:LYS:O	2.10	0.52
1:A:208:ASP:HB2	1:A:237:LYS:HE2	1.92	0.52
1:B:495:ARG:HG2	1:B:525:MET:O	2.09	0.52
1:A:234:ARG:NH2	1:A:252:SER:O	2.42	0.52
1:A:173:HIS:O	1:A:175:PRO:HD3	2.10	0.52
1:A:555:CYS:O	1:A:586:LYS:HB2	2.10	0.51
1:B:114:CYS:SG	1:B:134:ARG:HD3	2.50	0.51
1:A:232:ILE:O	1:A:232:ILE:HG23	2.10	0.51
1:B:118:ASN:O	1:B:122:PHE:HA	2.09	0.51
1:B:308:ASN:HD22	1:B:309:LEU:N	2.08	0.51
1:A:75:LYS:HD3	2:A:2106:HOH:O	2.10	0.51
1:A:323:GLN:HB3	1:A:337:TYR:HB2	1.91	0.51
1:A:517:PRO:HB2	1:A:520:GLY:HA3	1.93	0.51
1:A:320:LYS:HD3	2:A:2279:HOH:O	2.11	0.51
1:A:301:LEU:HD21	1:A:395:LYS:HG2	1.93	0.51
1:B:320:LYS:HE3	2:B:2039:HOH:O	2.10	0.51
1:A:103:TYR:HE2	1:A:152:LEU:HD22	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:TYR:N	1:B:621:HIS:O	2.33	0.50
1:A:433:LEU:O	1:A:434:GLU:C	2.50	0.50
1:B:333:LYS:HE2	1:B:335:VAL:CG1	2.40	0.50
1:B:63:GLU:HG3	1:B:65:TYR:HE2	1.76	0.50
1:A:118:ASN:O	1:A:122:PHE:N	2.44	0.50
1:B:435:HIS:ND1	1:B:435:HIS:N	2.57	0.50
1:A:343:LYS:C	1:A:343:LYS:HD3	2.32	0.50
1:B:584:GLY:O	1:B:585:ARG:O	2.29	0.50
1:A:45:ALA:O	1:A:91:ILE:HG12	2.12	0.50
1:A:608:ARG:CD	1:A:608:ARG:N	2.54	0.50
1:B:545:PHE:HB3	1:B:593:LEU:CD1	2.41	0.50
1:A:503:PRO:N	1:A:504:PRO:HD2	2.26	0.50
1:B:512:HIS:HD2	2:B:2156:HOH:O	1.94	0.50
1:A:134:ARG:HH21	1:A:170:ASN:HB3	1.76	0.50
1:A:193:ALA:HA	1:A:211:TYR:O	2.12	0.50
1:A:583:MET:O	1:A:587:ASN:HB2	2.12	0.50
1:A:543:HIS:HB2	1:A:623:LEU:HD13	1.93	0.49
1:B:537:LYS:HG2	2:B:2442:HOH:O	2.12	0.49
1:B:535:LYS:O	1:B:537:LYS:CE	2.60	0.49
1:B:322:MET:HE3	2:B:2304:HOH:O	2.12	0.49
1:B:279:ARG:HD2	2:B:2240:HOH:O	2.13	0.49
1:B:209:ARG:NE	2:B:2193:HOH:O	2.44	0.49
1:A:103:TYR:CE2	1:A:152:LEU:HD22	2.48	0.49
1:B:196:ILE:HG22	1:B:198:LYS:CE	2.43	0.49
1:B:199:SER:HB3	1:B:200:PRO:CA	2.40	0.49
1:B:72:LYS:HA	1:B:75:LYS:HB3	1.93	0.48
1:B:582:LEU:HA	1:B:587:ASN:O	2.13	0.48
1:A:390:PRO:HG2	1:A:393:ILE:HD11	1.94	0.48
1:A:322:MET:HG3	1:A:380:ASP:HA	1.94	0.48
1:A:391:ARG:NH1	1:A:391:ARG:CG	2.75	0.48
1:B:118:ASN:O	1:B:122:PHE:CA	2.62	0.48
1:A:38:LYS:HG2	1:A:459:SER:OG	2.12	0.48
1:B:357:ALA:O	1:B:358:ASN:HB2	2.14	0.48
1:B:403:VAL:HG23	1:B:419:PHE:HB2	1.96	0.48
1:B:14:ARG:HG3	2:B:2008:HOH:O	2.13	0.48
1:A:577:SER:CB	1:A:578:PRO:HA	2.44	0.48
1:A:34:LEU:HD13	1:A:41:LEU:CD1	2.44	0.48
1:B:69:SER:O	1:B:73:LYS:HB2	2.13	0.48
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.14	0.48
1:B:544:PHE:HB3	1:B:626:LYS:HZ2	1.78	0.48
1:B:398:ASN:ND2	2:B:2325:HOH:O	2.37	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:O	1:A:355:ARG:HB2	2.14	0.48
1:A:267:LEU:HD23	1:B:297:ASN:HA	1.94	0.48
1:A:591:PHE:HD1	1:B:550:THR:HG21	1.79	0.48
1:A:517:PRO:O	1:A:520:GLY:N	2.47	0.48
1:A:626:LYS:O	1:A:627:VAL:HB	2.14	0.48
1:A:392:LEU:C	1:A:392:LEU:HD23	2.34	0.48
1:A:308:ASN:ND2	2:A:2242:HOH:O	2.43	0.48
1:B:460:LYS:H	1:B:464:ARG:HH21	1.60	0.47
1:A:336:ARG:HD2	1:A:338:ASN:ND2	2.28	0.47
1:A:198:LYS:HB2	2:A:2127:HOH:O	2.14	0.47
1:A:301:LEU:HD23	1:A:395:LYS:HA	1.95	0.47
1:B:62:HIS:HB3	1:B:122:PHE:CD2	2.50	0.47
1:B:169:ARG:O	1:B:175:PRO:HA	2.14	0.47
1:B:572:VAL:O	1:B:572:VAL:HG23	2.15	0.47
1:B:196:ILE:HG22	1:B:198:LYS:HE2	1.96	0.47
1:B:600:VAL:HA	1:B:621:HIS:O	2.15	0.47
1:B:138:ASP:HB3	1:B:141:HIS:CG	2.49	0.47
1:B:556:SER:O	1:B:618:VAL:HG13	2.15	0.47
1:A:609:VAL:HG12	1:A:612:LYS:O	2.14	0.47
1:A:343:LYS:O	1:A:345:ARG:N	2.47	0.47
1:A:391:ARG:NH1	1:A:391:ARG:HG2	2.29	0.47
1:A:230:PRO:HB3	1:A:272:LEU:HB2	1.97	0.47
1:B:391:ARG:HD3	1:B:391:ARG:HA	1.76	0.47
1:B:460:LYS:O	1:B:461:LYS:HG2	2.15	0.47
1:A:261:SER:HB2	1:A:267:LEU:O	2.15	0.46
1:A:515:GLU:O	1:A:516:SER:O	2.33	0.46
1:B:59:GLU:OE1	1:B:59:GLU:HA	2.15	0.46
1:A:84:GLN:OE1	1:A:84:GLN:HA	2.15	0.46
1:A:86:GLU:HB3	1:A:110:PHE:HE2	1.79	0.46
1:A:100:THR:HG23	1:A:100:THR:O	2.14	0.46
1:B:47:GLU:OE2	1:B:67:LYS:HB3	2.15	0.46
1:A:517:PRO:O	1:A:518:SER:C	2.54	0.46
1:B:118:ASN:ND2	2:B:2100:HOH:O	2.49	0.46
1:A:346:PRO:HG2	1:A:372:PHE:CD2	2.50	0.46
1:A:495:ARG:CG	1:A:495:ARG:NH1	2.63	0.46
1:B:555:CYS:HB2	1:B:566:TRP:CZ2	2.50	0.46
1:A:608:ARG:NH1	1:A:608:ARG:HG3	2.29	0.46
1:A:108:ASN:HB3	1:A:111:GLN:O	2.15	0.46
1:B:495:ARG:HD2	2:B:2386:HOH:O	2.16	0.46
1:B:446:PHE:CE1	1:B:475:VAL:HG23	2.50	0.46
1:B:281:PRO:HB3	2:B:2247:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:NH1	2:A:2212:HOH:O	2.49	0.45
1:A:188:PRO:HA	1:A:215:THR:O	2.16	0.45
1:A:320:LYS:HE3	1:A:336:ARG:HH11	1.82	0.45
1:B:598:SER:OG	1:B:624:GLU:HA	2.16	0.45
1:A:181:ALA:HB1	1:A:183:PRO:HD2	1.98	0.45
1:A:151:GLU:OE1	1:A:171:SER:HB3	2.17	0.45
1:A:92:ARG:HD2	1:A:143:TYR:CE2	2.52	0.45
1:A:503:PRO:CD	1:A:504:PRO:HD2	2.47	0.45
1:B:536:SER:O	1:B:537:LYS:O	2.34	0.45
1:B:196:ILE:O	1:B:198:LYS:HE3	2.17	0.45
1:B:581:GLY:O	1:B:589:LEU:HD12	2.16	0.45
1:A:524:GLU:CG	1:A:531:VAL:HG21	2.47	0.44
1:A:528:ASP:O	1:A:531:VAL:HG22	2.17	0.44
1:A:37:ASP:O	1:A:38:LYS:HB2	2.17	0.44
1:A:343:LYS:O	1:A:344:PRO:C	2.51	0.44
1:B:47:GLU:CD	1:B:67:LYS:HA	2.38	0.44
1:B:370:LEU:HD11	2:B:2289:HOH:O	2.18	0.44
1:B:608:ARG:NH1	2:B:2435:HOH:O	2.35	0.44
1:A:262:ARG:HA	2:A:2220:HOH:O	2.17	0.44
1:A:100:THR:HG23	2:A:2134:HOH:O	2.18	0.44
1:A:420:VAL:O	1:A:420:VAL:HG23	2.18	0.44
1:A:247:GLN:O	1:A:248:LYS:HB2	2.17	0.44
1:B:63:GLU:HG3	1:B:65:TYR:CE2	2.52	0.44
1:A:489:GLU:O	1:A:493:LEU:HD12	2.18	0.44
1:A:504:PRO:CD	1:A:517:PRO:HG3	2.48	0.44
1:B:328:GLU:HB3	2:B:2266:HOH:O	2.18	0.44
1:A:446:PHE:CE1	1:A:475:VAL:HG23	2.53	0.44
1:A:576:GLU:OE1	1:A:577:SER:O	2.36	0.44
1:B:324:SER:HB2	1:B:334:TRP:CZ2	2.53	0.44
1:A:516:SER:O	1:A:518:SER:N	2.50	0.44
1:A:593:LEU:HA	1:A:593:LEU:HD12	1.84	0.44
1:A:543:HIS:HB2	1:A:623:LEU:CD1	2.47	0.44
1:B:153:TYR:CZ	1:B:169:ARG:HD3	2.53	0.44
1:A:526:SER:O	1:A:610:LYS:HB2	2.18	0.43
1:A:609:VAL:CG2	1:A:610:LYS:N	2.67	0.43
1:B:573:LEU:HD23	1:B:573:LEU:O	2.17	0.43
1:B:154:SER:O	1:B:167:ILE:HA	2.18	0.43
1:A:123:LYS:HD3	2:A:2137:HOH:O	2.18	0.43
1:A:595:GLU:HA	1:A:625:VAL:CG1	2.48	0.43
1:A:28:ASN:HA	1:A:471:ASN:HA	1.99	0.43
1:B:395:LYS:HZ2	1:B:395:LYS:HB3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:SER:OG	1:A:625:VAL:HG12	2.18	0.43
1:B:262:ARG:HD2	1:B:389:ARG:NH1	2.33	0.43
1:B:336:ARG:NE	1:B:380:ASP:OD2	2.48	0.43
1:B:13:HIS:HB3	2:B:2008:HOH:O	2.19	0.43
1:B:301:LEU:HD11	1:B:395:LYS:HG3	2.00	0.43
1:A:102:LEU:HG	1:A:119:LEU:HD21	2.00	0.43
1:B:12:GLU:HB2	1:B:14:ARG:HD3	2.00	0.43
1:A:503:PRO:HD2	1:A:504:PRO:HD2	2.01	0.43
1:A:564:VAL:HG21	2:A:2389:HOH:O	2.18	0.43
1:B:562:ALA:HB2	1:B:607:GLU:HG3	2.01	0.43
1:A:333:LYS:HG3	1:B:333:LYS:NZ	2.34	0.42
1:B:394:LYS:HG2	1:B:397:VAL:HG11	2.00	0.42
1:B:14:ARG:H	1:B:14:ARG:HG3	1.62	0.42
1:A:516:SER:CB	1:A:517:PRO:HD2	2.44	0.42
1:A:517:PRO:O	1:A:521:LEU:HG	2.20	0.42
1:A:408:GLN:HG2	1:A:412:GLY:O	2.19	0.42
1:A:354:ALA:O	1:A:359:TYR:HB2	2.19	0.42
1:B:567:LYS:HG2	1:B:572:VAL:HA	2.01	0.42
1:B:446:PHE:HB3	1:B:448:ASP:OD1	2.19	0.42
1:A:421:SER:HB2	1:A:452:VAL:HB	2.01	0.42
1:A:563:ARG:HA	2:A:2383:HOH:O	2.19	0.42
1:B:463:ASN:HA	1:B:463:ASN:HD22	1.61	0.42
1:A:241:GLY:HA2	1:A:249:LYS:O	2.20	0.42
1:B:464:ARG:NH1	1:B:479:LEU:HD11	2.35	0.42
1:B:327:VAL:O	1:B:328:GLU:HB2	2.19	0.42
1:A:450:GLU:OE2	1:A:451:PRO:HD2	2.19	0.42
1:A:62:HIS:NE2	2:A:2088:HOH:O	2.36	0.42
1:B:345:ARG:HA	1:B:346:PRO:HD3	1.96	0.42
1:B:13:HIS:ND1	1:B:447:GLN:HG2	2.34	0.42
1:A:118:ASN:ND2	2:A:2135:HOH:O	2.52	0.42
1:A:92:ARG:HD2	1:A:143:TYR:CZ	2.55	0.42
1:A:46:ARG:O	1:A:47:GLU:HB2	2.19	0.42
1:B:285:VAL:O	1:B:285:VAL:HG13	2.20	0.42
1:A:582:LEU:CD2	1:A:585:ARG:HA	2.49	0.42
1:A:534:ASP:CG	1:A:535:LYS:N	2.73	0.42
1:B:532:CYS:HB2	1:B:535:LYS:HE2	2.01	0.41
1:B:116:HIS:CE1	1:B:127:LYS:HE3	2.55	0.41
1:A:34:LEU:HD13	1:A:41:LEU:HD13	2.02	0.41
1:A:225:PHE:HE2	1:A:296:LEU:CD2	2.33	0.41
1:A:513:GLN:HG3	1:A:514:THR:N	2.36	0.41
1:A:68:VAL:HG21	1:A:87:CYS:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:C	1:A:526:SER:H	2.23	0.41
1:B:552:GLU:HG3	1:B:552:GLU:H	1.78	0.41
1:A:240:GLN:HB2	1:A:362:SER:OG	2.19	0.41
1:B:503:PRO:CD	1:B:504:PRO:HD2	2.51	0.41
1:A:408:GLN:NE2	1:A:412:GLY:O	2.51	0.41
1:B:182:ILE:HD11	2:B:2172:HOH:O	2.19	0.41
1:B:329:GLN:O	1:B:330:SER:CB	2.68	0.41
1:B:148:VAL:HG22	1:B:195:VAL:HG22	2.02	0.41
1:B:563:ARG:HG2	2:B:2189:HOH:O	2.21	0.41
1:A:565:PHE:CD1	1:A:565:PHE:N	2.88	0.41
1:B:280:SER:HA	1:B:281:PRO:HD3	1.96	0.41
1:A:154:SER:O	1:A:167:ILE:HA	2.20	0.41
1:A:12:GLU:H	1:A:15:GLU:CG	2.34	0.41
1:A:551:ALA:O	1:A:589:LEU:HA	2.20	0.41
1:A:138:ASP:HB3	1:A:141:HIS:CG	2.55	0.41
1:B:625:VAL:O	1:B:625:VAL:HG22	2.21	0.41
1:B:532:CYS:HA	1:B:533:PRO:HD3	1.94	0.41
1:B:604:LEU:HD22	1:B:617:VAL:HG22	2.02	0.41
1:A:333:LYS:CD	1:B:333:LYS:HD3	2.51	0.41
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.75	0.41
1:B:395:LYS:NZ	1:B:395:LYS:HB3	2.36	0.41
1:B:353:GLU:H	1:B:353:GLU:HG2	1.65	0.41
1:B:187:GLU:HA	2:B:2142:HOH:O	2.20	0.41
1:A:182:ILE:HA	1:A:182:ILE:HD12	1.86	0.41
1:A:608:ARG:CG	1:A:608:ARG:NH1	2.84	0.41
1:B:346:PRO:HG2	1:B:372:PHE:CD2	2.56	0.41
1:B:24:PRO:O	1:B:25:ASP:HB2	2.21	0.41
1:B:98:SER:HB2	2:B:2085:HOH:O	2.21	0.41
1:A:131:GLY:O	1:A:134:ARG:HG3	2.21	0.40
1:B:281:PRO:HA	2:B:2244:HOH:O	2.20	0.40
1:A:610:LYS:HG3	2:A:2359:HOH:O	2.20	0.40
1:B:583:MET:HB3	1:B:587:ASN:HB2	2.03	0.40
1:A:229:ILE:HA	1:A:230:PRO:HD3	1.91	0.40
1:A:543:HIS:NE2	1:A:621:HIS:ND1	2.55	0.40
1:B:434:GLU:OE2	1:B:610:LYS:HE3	2.22	0.40
1:A:333:LYS:HZ3	1:B:333:LYS:HB2	1.84	0.40
1:B:231:ARG:NH1	1:B:257:ARG:HG3	2.36	0.40
1:B:484:LYS:HD2	2:B:2009:HOH:O	2.20	0.40
1:A:609:VAL:HG13	1:A:610:LYS:N	2.36	0.40
1:B:70:GLU:OE1	1:B:83:LYS:NZ	2.48	0.40
1:B:29:TYR:CD2	1:B:473:GLY:HA2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:HD11	1:B:399:TYR:HB2	2.03	0.40
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.77	0.40
1:B:577:SER:CB	1:B:578:PRO:HA	2.51	0.40
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.82	0.40
1:A:155:GLY:O	1:A:156:THR:HB	2.22	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	618/663 (93%)	565 (91%)	35 (6%)	18 (3%)	6	2
1	B	618/663 (93%)	567 (92%)	38 (6%)	13 (2%)	9	3
All	All	1236/1326 (93%)	1132 (92%)	73 (6%)	31 (2%)	7	2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	A	511	LEU
1	A	516	SER
1	A	610	LYS
1	B	199	SER
1	B	280	SER
1	B	343	LYS
1	B	537	LYS
1	B	585	ARG
1	B	586	LYS
1	B	610	LYS
1	A	326	THR
1	A	435	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	512	HIS
1	A	513	GLN
1	A	517	PRO
1	A	582	LEU
1	A	586	LYS
1	A	609	VAL
1	A	627	VAL
1	B	593	LEU
1	A	549	GLY
1	B	594	SER
1	A	328	GLU
1	B	538	GLY
1	B	569	GLN
1	B	575	ALA
1	A	331	HIS
1	A	343	LYS
1	B	342	PRO
1	A	300	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	545/582 (94%)	471 (86%)	74 (14%)	5	2
1	B	545/582 (94%)	465 (85%)	80 (15%)	4	2
All	All	1090/1164 (94%)	936 (86%)	154 (14%)	4	2

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	34	LEU
1	A	36	GLU
1	A	38	LYS
1	A	72	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	SER
1	A	88	LEU
1	A	97	LEU
1	A	100	THR
1	A	132	LYS
1	A	173	HIS
1	A	174	SER
1	A	182	ILE
1	A	195	VAL
1	A	197	ARG
1	A	198	LYS
1	A	209	ARG
1	A	225	PHE
1	A	227	VAL
1	A	234	ARG
1	A	244	ARG
1	A	245	THR
1	A	249	LYS
1	A	264	ASP
1	A	265	SER
1	A	283	LEU
1	A	314	GLU
1	A	320	LYS
1	A	323	GLN
1	A	330	SER
1	A	332	THR
1	A	333	LYS
1	A	343	LYS
1	A	352	SER
1	A	358	ASN
1	A	361	SER
1	A	389	ARG
1	A	391	ARG
1	A	392	LEU
1	A	432	SER
1	A	433	LEU
1	A	435	HIS
1	A	457	LEU
1	A	461	LYS
1	A	495	ARG
1	A	511	LEU
1	A	513	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	SER
1	A	519	ARG
1	A	530	SER
1	A	534	ASP
1	A	535	LYS
1	A	537	LYS
1	A	541	ARG
1	A	542	GLN
1	A	546	LYS
1	A	552	GLU
1	A	556	SER
1	A	557	GLN
1	A	563	ARG
1	A	564	VAL
1	A	567	LYS
1	A	573	LEU
1	A	576	GLU
1	A	577	SER
1	A	579	LYS
1	A	582	LEU
1	A	593	LEU
1	A	605	SER
1	A	606	GLU
1	A	607	GLU
1	A	608	ARG
1	A	610	LYS
1	A	626	LYS
1	B	14	ARG
1	B	15	GLU
1	B	17	HIS
1	B	36	GLU
1	B	38	LYS
1	B	47	GLU
1	B	59	GLU
1	B	60	LYS
1	B	68	VAL
1	B	72	LYS
1	B	73	LYS
1	B	75	LYS
1	B	82	SER
1	B	83	LYS
1	B	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	ARG
1	B	111	GLN
1	B	172	SER
1	B	174	SER
1	B	195	VAL
1	B	198	LYS
1	B	206	GLU
1	B	209	ARG
1	B	222	GLU
1	B	223	PHE
1	B	225	PHE
1	B	226	ARG
1	B	234	ARG
1	B	264	ASP
1	B	265	SER
1	B	272	LEU
1	B	278	LEU
1	B	283	LEU
1	B	301	LEU
1	B	308	ASN
1	B	323	GLN
1	B	328	GLU
1	B	329	GLN
1	B	330	SER
1	B	332	THR
1	B	333	LYS
1	B	343	LYS
1	B	353	GLU
1	B	355	ARG
1	B	392	LEU
1	B	395	LYS
1	B	435	HIS
1	B	447	GLN
1	B	459	SER
1	B	460	LYS
1	B	464	ARG
1	B	495	ARG
1	B	537	LYS
1	B	541	ARG
1	B	542	GLN
1	B	550	THR
1	B	552	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	557	GLN
1	B	563	ARG
1	B	564	VAL
1	B	569	GLN
1	B	570	ASN
1	B	573	LEU
1	B	574	LYS
1	B	577	SER
1	B	579	LYS
1	B	582	LEU
1	B	585	ARG
1	B	592	ASN
1	B	595	GLU
1	B	598	SER
1	B	604	LEU
1	B	610	LYS
1	B	612	LYS
1	B	613	THR
1	B	620	LYS
1	B	623	LEU
1	B	625	VAL
1	B	626	LYS
1	B	627	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	323	GLN
1	A	338	ASN
1	A	471	ASN
1	A	513	GLN
1	A	557	GLN
1	A	592	ASN
1	B	13	HIS
1	B	308	ASN
1	B	331	HIS
1	B	338	ASN
1	B	364	ASN
1	B	401	GLN
1	B	408	GLN
1	B	447	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	463	ASN
1	B	471	ASN
1	B	513	GLN
1	B	547	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

6.1 Protein, DNA and RNA chains

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	622/663 (93%)	0.03	36 (5%) 26 28	13, 36, 81, 100	0
1	B	622/663 (93%)	-0.02	47 (7%) 17 18	8, 29, 85, 100	0
All	All	1244/1326 (93%)	0.00	83 (6%) 21 22	8, 33, 84, 100	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	8.6
1	A	327	VAL	8.3
1	B	577	SER	8.0
1	A	628	VAL	7.9
1	A	199	SER	7.2
1	B	584	GLY	6.5
1	B	200	PRO	6.4
1	A	283	LEU	6.2
1	A	519	ARG	6.1
1	A	515	GLU	6.0
1	A	326	THR	5.4
1	B	626	LYS	5.3
1	A	514	THR	5.1
1	A	328	GLU	5.0
1	B	327	VAL	5.0
1	B	627	VAL	4.8
1	A	518	SER	4.7
1	B	537	LYS	4.6
1	A	585	ARG	4.3
1	B	199	SER	4.2
1	A	627	VAL	4.2
1	B	585	ARG	4.1
1	A	435	HIS	4.1
1	B	435	HIS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	329	GLN	4.0
1	B	282	GLY	3.9
1	B	624	GLU	3.9
1	B	544	PHE	3.9
1	A	173	HIS	3.7
1	B	37	ASP	3.6
1	B	578	PRO	3.6
1	B	84	GLN	3.5
1	A	198	LYS	3.4
1	B	328	GLU	3.4
1	A	331	HIS	3.1
1	B	283	LEU	3.0
1	B	71	ASP	3.0
1	B	570	ASN	3.0
1	A	343	LYS	2.9
1	B	592	ASN	2.8
1	A	281	PRO	2.8
1	A	520	GLY	2.8
1	B	611	ASN	2.8
1	B	460	LYS	2.7
1	B	326	THR	2.7
1	B	281	PRO	2.7
1	B	628	VAL	2.7
1	B	576	GLU	2.6
1	B	572	VAL	2.6
1	A	205	GLY	2.6
1	B	459	SER	2.5
1	B	590	ILE	2.5
1	B	625	VAL	2.5
1	A	330	SER	2.5
1	B	588	LEU	2.4
1	A	282	GLY	2.4
1	A	172	SER	2.4
1	B	551	ALA	2.4
1	A	578	PRO	2.4
1	A	434	GLU	2.4
1	A	244	ARG	2.4
1	A	99	ALA	2.4
1	B	17	HIS	2.4
1	A	284	LYS	2.3
1	B	610	LYS	2.3
1	B	538	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	517	PRO	2.3
1	B	264	ASP	2.3
1	B	596	GLY	2.2
1	B	609	VAL	2.2
1	B	623	LEU	2.2
1	A	356	ALA	2.2
1	B	461	LYS	2.2
1	B	356	ALA	2.1
1	B	14	ARG	2.1
1	A	264	ASP	2.1
1	B	463	ASN	2.1
1	A	576	GLU	2.1
1	B	173	HIS	2.1
1	A	592	ASN	2.1
1	B	99	ALA	2.0
1	A	355	ARG	2.0
1	B	462	GLY	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.