Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:36 PM GMT

PDB ID	:	1BM0
Title	:	CRYSTAL STRUCTURE OF HUMAN SERUM ALBUMIN
Authors	:	Sugio, S.; Kashima, A.; Mochizuki, S.; Noda, M.; Kobayashi, K.
Deposited on	:	1998-07-28
Resolution	:	2.50 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:

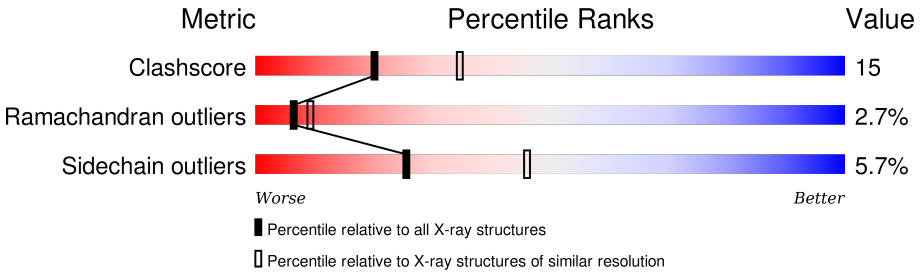
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	585	63% 32%
1	B	585	64% 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9202 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 SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			
1	B	578	Total	C	N	O	S	0	0	0
			4599	2903	776	879	41			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	3	Total	O	0	0
			3	3		

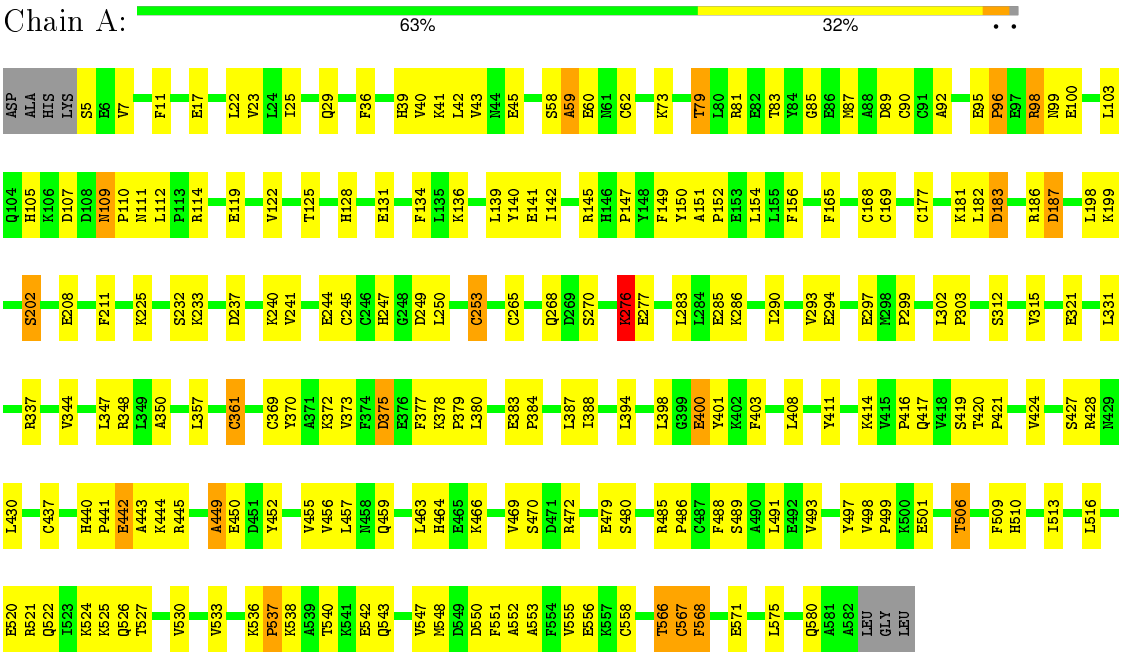
3 Residue-property plots (i)

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.

Note EDS was not executed.

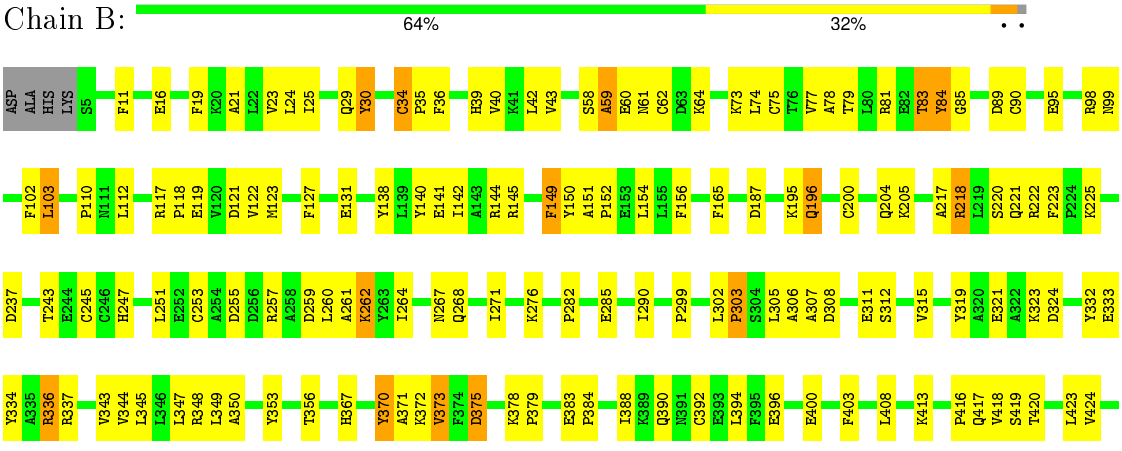
- Molecule 1: SERUM ALBUMIN

Chain A:



- Molecule 1: SERUM ALBUMIN

Chain B:




S427
R428
S435
K436
C437
C438
K439
H440
P441
E442
A443
K444
C448
A449
Y452
L453
L457
L460
H464
E465
S470
D471
R472
V473
T474
K475
E479
N483
P486
L491
V498
E501
T515
R521
K525
A528
L529
L532
V533
K534
H535
K536
P537
K538
A539
T540
Q543
L544
K545
A546
V547
M548
F551
V555
K564
E565
T566
C567
F568
E571
L575
Q580
A581
A582
LEU
GLY
LEU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.36Å 96.89Å 59.24Å 91.04° 103.40° 74.94°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	77.1 (50.00-2.50)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.207 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.67	0/4688	0.84	2/6324 (0.0%)
1	B	0.67	0/4688	0.82	1/6324 (0.0%)
All	All	0.67	0/9376	0.83	3/12648 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	98	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	369	CYS	CA-CB-SG	5.05	123.09	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	332	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4599	0	4518	142	0
1	B	4599	0	4518	126	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
All	All	9202	0	9036	268	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 15.

All (268) 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:417:GLN:HB3	1:A:469:VAL:HG12	1.44	0.99
1:A:156:PHE:HE1	1:A:285:GLU:HG3	1.34	0.91
1:A:240:LYS:O	1:A:244:GLU:HG3	1.73	0.88
1:A:370:TYR:O	1:A:373:VAL:HG23	1.75	0.87
1:A:417:GLN:HB2	1:A:470:SER:HB3	1.58	0.85
1:B:119:GLU:HB2	1:B:122:VAL:HG23	1.61	0.82
1:A:424:VAL:O	1:A:428:ARG:HG3	1.79	0.82
1:A:36:PHE:O	1:A:40:VAL:HG23	1.82	0.80
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.23	0.79
1:A:41:LYS:HZ2	1:A:42:LEU:HD23	1.47	0.79
1:A:151:ALA:HB2	1:A:250:LEU:HD13	1.65	0.77
1:B:90:CYS:O	1:B:98:ARG:HG3	1.85	0.77
1:B:42:LEU:HD22	1:B:73:LYS:HG3	1.68	0.75
1:B:571:GLU:O	1:B:575:LEU:HG	1.87	0.75
1:A:156:PHE:CE1	1:A:285:GLU:HG3	2.22	0.74
1:B:200:CYS:O	1:B:204:GLN:HG3	1.86	0.74
1:A:119:GLU:HB2	1:A:122:VAL:HG23	1.70	0.74
1:B:420:THR:O	1:B:424:VAL:HG23	1.88	0.73
1:A:525:LYS:HE2	1:A:552:ALA:HA	1.71	0.72
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.71	0.72
1:B:307:ALA:HA	1:B:311:GLU:HB2	1.70	0.72
1:B:356:THR:HG21	1:B:373:VAL:HG22	1.70	0.72
1:B:418:VAL:HB	1:B:423:LEU:HD21	1.70	0.71
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.05	0.71
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.26	0.71
1:A:81:ARG:HB2	1:A:85:GLY:HA2	1.75	0.69
1:A:464:HIS:HE1	1:A:470:SER:H	1.41	0.69
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:HE1	1:B:285:GLU:HG3	1.57	0.68
1:A:312:SER:O	1:A:315:VAL:HG23	1.93	0.68
1:A:384:PRO:O	1:A:388:ILE:HG12	1.93	0.68
1:B:303:PRO:HG2	1:B:337:ARG:HH22	1.59	0.67
1:A:225:LYS:HZ1	1:A:297:GLU:HB2	1.61	0.66
1:A:498:VAL:HG13	1:A:498:VAL:O	1.95	0.65
1:B:218:ARG:HH21	1:B:221:GLN:HB2	1.62	0.65
1:A:268:GLN:OE1	1:A:276:LYS:HA	1.97	0.64
1:A:387:LEU:HD22	1:A:485:ARG:HH11	1.62	0.64
1:B:149:PHE:HD1	1:B:150:TYR:N	1.96	0.64
1:B:319:TYR:O	1:B:323:LYS:HB3	1.98	0.64
1:A:141:GLU:HB3	1:A:145:ARG:NH1	2.12	0.64
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.80	0.63
1:B:543:GLN:O	1:B:546:ALA:HB3	1.98	0.63
1:A:388:ILE:HD12	1:A:449:ALA:HB1	1.81	0.63
1:B:83:THR:HB	1:B:84:TYR:CE1	2.34	0.63
1:B:370:TYR:O	1:B:373:VAL:HG23	1.98	0.63
1:B:259:ASP:O	1:B:262:LYS:HB3	1.99	0.63
1:A:141:GLU:HB3	1:A:145:ARG:HH12	1.64	0.62
1:A:571:GLU:O	1:A:575:LEU:HG	1.99	0.62
1:A:5:SER:HA	1:A:62:CYS:O	2.00	0.62
1:A:177:CYS:O	1:A:181:LYS:HD2	2.00	0.61
1:A:41:LYS:NZ	1:A:42:LEU:HD23	2.15	0.61
1:B:312:SER:O	1:B:315:VAL:HG23	2.02	0.60
1:B:25:ILE:HD13	1:B:154:LEU:HD23	1.83	0.60
1:B:413:LYS:O	1:B:416:PRO:HD3	2.00	0.60
1:B:475:LYS:O	1:B:479:GLU:HB2	2.02	0.59
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.83	0.59
1:A:394:LEU:HD11	1:A:398:LEU:HD11	1.85	0.59
1:A:373:VAL:HG12	1:A:377:PHE:CE1	2.38	0.59
1:B:25:ILE:CD1	1:B:154:LEU:HD23	2.33	0.58
1:B:417:GLN:HB2	1:B:470:SER:HB2	1.84	0.58
1:B:528:ALA:O	1:B:532:LEU:HG	2.04	0.58
1:B:225:LYS:HG2	1:B:299:PRO:HG3	1.85	0.58
1:B:472:ARG:CZ	1:B:491:LEU:HD22	2.34	0.57
1:A:419:SER:OG	1:A:421:PRO:HD2	2.04	0.57
1:A:440:HIS:HB3	1:A:444:LYS:HB2	1.87	0.57
1:B:372:LYS:O	1:B:375:ASP:HB2	2.04	0.57
1:A:265:CYS:O	1:A:268:GLN:HB2	2.05	0.57
1:B:222:ARG:HG2	1:B:223:PHE:CE1	2.40	0.57
1:A:414:LYS:HD2	1:A:491:LEU:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PRO:HB2	1:A:302:LEU:HG	1.87	0.56
1:B:319:TYR:CD1	1:B:323:LYS:HB2	2.40	0.56
1:B:268:GLN:OE1	1:B:276:LYS:HA	2.06	0.56
1:A:276:LYS:HD3	1:A:277:GLU:HG3	1.88	0.56
1:A:552:ALA:O	1:A:556:GLU:HG2	2.05	0.56
1:B:110:PRO:HB2	1:B:112:LEU:HG	1.87	0.55
1:B:384:PRO:O	1:B:388:ILE:HG12	2.07	0.55
1:B:39:HIS:O	1:B:43:VAL:HG23	2.04	0.55
1:B:19:PHE:O	1:B:23:VAL:HG23	2.07	0.55
1:B:112:LEU:HD22	1:B:144:ARG:HH21	1.71	0.55
1:B:551:PHE:O	1:B:555:VAL:HG23	2.07	0.54
1:B:498:VAL:O	1:B:498:VAL:HG13	2.06	0.54
1:B:99:ASN:O	1:B:102:PHE:N	2.40	0.54
1:A:464:HIS:CE1	1:A:470:SER:H	2.23	0.54
1:A:25:ILE:O	1:A:29:GLN:HG3	2.08	0.54
1:A:225:LYS:NZ	1:A:297:GLU:HB2	2.22	0.53
1:A:103:LEU:HD11	1:A:247:HIS:CD2	2.44	0.53
1:B:61:ASN:HB3	1:B:64:LYS:HD2	1.89	0.53
1:B:251:LEU:O	1:B:255:ASP:HB2	2.09	0.53
1:A:459:GLN:O	1:A:463:LEU:HG	2.09	0.53
1:B:449:ALA:O	1:B:453:LEU:HG	2.08	0.53
1:B:567:CYS:O	1:B:571:GLU:HB2	2.09	0.53
1:A:497:TYR:O	1:A:499:PRO:HD3	2.09	0.53
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.91	0.52
1:A:378:LYS:HB2	1:A:379:PRO:HD3	1.91	0.52
1:A:516:LEU:O	1:A:521:ARG:NH2	2.42	0.52
1:B:119:GLU:HB2	1:B:122:VAL:CG2	2.36	0.52
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.92	0.52
1:B:333:GLU:O	1:B:336:ARG:HG2	2.09	0.52
1:A:81:ARG:C	1:A:83:THR:H	2.13	0.51
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.92	0.51
1:A:344:VAL:HG21	1:A:450:GLU:HG2	1.92	0.51
1:B:533:VAL:O	1:B:537:PRO:HG3	2.10	0.51
1:B:30:TYR:HD2	1:B:74:LEU:HD11	1.76	0.51
1:A:286:LYS:O	1:A:290:ILE:HG13	2.11	0.51
1:A:247:HIS:O	1:A:247:HIS:CG	2.63	0.51
1:B:521:ARG:O	1:B:525:LYS:HD3	2.11	0.51
1:A:303:PRO:HG2	1:A:337:ARG:HH22	1.75	0.51
1:B:140:TYR:CE2	1:B:144:ARG:NH1	2.79	0.50
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.94	0.50
1:A:567:CYS:O	1:A:571:GLU:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:TYR:CE1	1:A:522:GLN:HB3	2.46	0.50
1:A:331:LEU:HD21	1:A:347:LEU:CD2	2.42	0.50
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.94	0.50
1:A:414:LYS:C	1:A:416:PRO:HD3	2.32	0.50
1:B:437:CYS:HA	1:B:440:HIS:HD2	1.77	0.50
1:A:87:MET:CE	1:A:105:HIS:HB3	2.42	0.50
1:B:343:VAL:O	1:B:347:LEU:HG	2.12	0.49
1:B:259:ASP:O	1:B:262:LYS:HE3	2.12	0.49
1:A:401:TYR:HE1	1:A:522:GLN:HB3	1.77	0.49
1:A:45:GLU:OE1	1:A:73:LYS:HD2	2.13	0.49
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.52	0.49
1:A:414:LYS:O	1:A:416:PRO:HD3	2.12	0.49
1:A:95:GLU:OE1	1:A:99:ASN:HB2	2.13	0.49
1:A:348:ARG:NH2	1:A:450:GLU:OE2	2.44	0.49
1:A:533:VAL:O	1:A:537:PRO:HG3	2.12	0.49
1:A:198:LEU:HD22	1:A:455:VAL:HG22	1.94	0.49
1:B:345:LEU:HD11	1:B:349:LEU:HD21	1.95	0.49
1:B:441:PRO:O	1:B:443:ALA:N	2.45	0.49
1:A:472:ARG:HE	1:A:491:LEU:HD22	1.78	0.48
1:B:112:LEU:CD2	1:B:144:ARG:HH21	2.26	0.48
1:A:441:PRO:O	1:A:443:ALA:N	2.47	0.48
1:B:448:CYS:O	1:B:452:TYR:HB2	2.13	0.48
1:A:430:LEU:HD23	1:A:456:VAL:HG11	1.96	0.48
1:A:25:ILE:HD13	1:A:154:LEU:HD23	1.96	0.48
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.48
1:A:90:CYS:O	1:A:98:ARG:HG3	2.14	0.48
1:B:237:ASP:HB3	1:B:260:LEU:HD13	1.95	0.48
1:B:149:PHE:CD1	1:B:150:TYR:N	2.79	0.47
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.14	0.47
1:A:96:PRO:O	1:A:100:GLU:HB2	2.14	0.47
1:A:244:GLU:O	1:A:249:ASP:N	2.47	0.47
1:B:95:GLU:OE1	1:B:95:GLU:HA	2.15	0.47
1:B:196:GLN:HA	1:B:196:GLN:HE21	1.80	0.47
1:B:424:VAL:O	1:B:428:ARG:HG3	2.14	0.47
1:B:306:ALA:O	1:B:311:GLU:N	2.48	0.47
1:B:77:VAL:O	1:B:84:TYR:CE1	2.68	0.47
1:A:39:HIS:O	1:A:43:VAL:HG23	2.14	0.47
1:B:138:TYR:O	1:B:142:ILE:HG12	2.14	0.47
1:B:149:PHE:HD1	1:B:150:TYR:H	1.63	0.47
1:B:464:HIS:HE1	1:B:470:SER:H	1.63	0.47
1:B:367:HIS:O	1:B:371:ALA:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLU:O	1:B:403:PHE:HB3	2.15	0.47
1:B:36:PHE:O	1:B:40:VAL:HG23	2.15	0.46
1:B:112:LEU:HD22	1:B:144:ARG:NH2	2.29	0.46
1:B:218:ARG:HA	1:B:218:ARG:HE	1.81	0.46
1:B:457:LEU:O	1:B:460:LEU:HB3	2.15	0.46
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.97	0.46
1:A:79:THR:O	1:A:79:THR:HG22	2.15	0.46
1:B:156:PHE:CE1	1:B:285:GLU:HG3	2.44	0.46
1:B:11:PHE:CZ	1:B:16:GLU:HB2	2.51	0.46
1:A:450:GLU:OE2	1:A:485:ARG:NE	2.49	0.46
1:B:150:TYR:OH	1:B:257:ARG:HD2	2.16	0.46
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.79	0.45
1:A:199:LYS:HG2	1:A:211:PHE:HE1	1.81	0.45
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.81	0.45
1:A:543:GLN:O	1:A:547:VAL:HG23	2.15	0.45
1:A:237:ASP:O	1:A:241:VAL:HG23	2.16	0.45
1:B:243:THR:O	1:B:247:HIS:HB2	2.16	0.45
1:A:377:PHE:O	1:A:380:LEU:HB2	2.16	0.45
1:A:331:LEU:HD21	1:A:347:LEU:HD23	1.99	0.45
1:A:408:LEU:HD11	1:A:526:GLN:HG2	1.99	0.45
1:A:414:LYS:HE2	1:A:414:LYS:HB2	1.59	0.45
1:A:536:LYS:O	1:A:536:LYS:HG2	2.17	0.45
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.57	0.45
1:A:542:GLU:HG3	1:A:543:GLN:N	2.32	0.44
1:B:564:LYS:O	1:B:565:GLU:HB2	2.17	0.44
1:B:282:PRO:HB2	1:B:285:GLU:OE1	2.18	0.44
1:B:21:ALA:O	1:B:25:ILE:HG13	2.18	0.44
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.99	0.44
1:A:131:GLU:O	1:A:134:PHE:HB3	2.17	0.44
1:A:7:VAL:O	1:A:11:PHE:HB2	2.18	0.44
1:A:165:PHE:O	1:A:169:CYS:SG	2.76	0.44
1:B:350:ALA:O	1:B:353:TYR:N	2.50	0.44
1:B:539:ALA:O	1:B:543:GLN:NE2	2.51	0.44
1:B:81:ARG:C	1:B:83:THR:H	2.21	0.44
1:B:267:ASN:O	1:B:271:ILE:HG13	2.18	0.44
1:B:392:CYS:O	1:B:396:GLU:HG2	2.18	0.44
1:B:262:LYS:C	1:B:262:LYS:HD2	2.38	0.44
1:A:125:THR:O	1:A:128:HIS:N	2.51	0.44
1:A:244:GLU:HB2	1:A:253:CYS:HB2	2.00	0.44
1:B:25:ILE:O	1:B:29:GLN:HG3	2.17	0.43
1:B:196:GLN:CA	1:B:196:GLN:HE21	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:CD	1:A:485:ARG:HH22	2.20	0.43
1:B:491:LEU:HA	1:B:491:LEU:HD23	1.71	0.43
1:A:400:GLU:O	1:A:403:PHE:HB3	2.19	0.43
1:A:372:LYS:O	1:A:375:ASP:HB2	2.19	0.43
1:A:150:TYR:CD1	1:A:152:PRO:HD2	2.53	0.43
1:B:378:LYS:HB3	1:B:378:LYS:HE3	1.77	0.43
1:A:109:ASN:C	1:A:109:ASN:HD22	2.22	0.43
1:B:127:PHE:CE1	1:B:131:GLU:HG3	2.54	0.43
1:A:107:ASP:O	1:A:147:PRO:HG3	2.19	0.43
1:A:498:VAL:CG1	1:A:498:VAL:O	2.66	0.43
1:A:513:ILE:HG21	1:A:568:PHE:HZ	1.84	0.43
1:B:217:ALA:O	1:B:220:SER:HB2	2.18	0.43
1:A:168:CYS:SG	1:A:177:CYS:C	2.97	0.42
1:A:408:LEU:HD23	1:A:427:SER:CB	2.49	0.42
1:B:305:LEU:HD13	1:B:334:TYR:CD2	2.53	0.42
1:A:357:LEU:O	1:A:361:CYS:HB2	2.19	0.42
1:A:550:ASP:O	1:A:553:ALA:HB3	2.20	0.42
1:A:268:GLN:OE1	1:A:276:LYS:CA	2.65	0.42
1:A:497:TYR:CD2	1:A:537:PRO:HG2	2.54	0.42
1:B:75:CYS:HA	1:B:78:ALA:HB3	2.01	0.42
1:B:348:ARG:NH2	1:B:486:PRO:HD3	2.34	0.42
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.85	0.42
1:A:437:CYS:HA	1:A:440:HIS:HD2	1.84	0.42
1:A:558:CYS:SG	1:A:567:CYS:C	2.98	0.42
1:A:513:ILE:HG21	1:A:568:PHE:CZ	2.55	0.42
1:B:536:LYS:HE3	1:B:540:THR:HG22	2.02	0.42
1:B:34:CYS:HB3	1:B:39:HIS:CE1	2.55	0.42
1:B:19:PHE:CD1	1:B:19:PHE:C	2.92	0.42
1:B:141:GLU:O	1:B:145:ARG:HD2	2.20	0.42
1:A:457:LEU:HD13	1:A:488:PHE:CD2	2.54	0.42
1:A:183:ASP:O	1:A:187:ASP:HB2	2.19	0.42
1:B:23:VAL:O	1:B:24:LEU:C	2.58	0.42
1:B:117:ARG:HA	1:B:118:PRO:HD3	1.87	0.42
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.89	0.42
1:A:420:THR:HG23	1:A:530:VAL:HG11	2.02	0.42
1:A:199:LYS:O	1:A:202:SER:HB2	2.20	0.42
1:A:551:PHE:O	1:A:555:VAL:HG23	2.20	0.42
1:A:344:VAL:CG2	1:A:450:GLU:HG2	2.49	0.42
1:A:408:LEU:HD23	1:A:427:SER:HB2	2.02	0.41
1:B:205:LYS:HE2	1:B:465:GLU:OE2	2.20	0.41
1:A:293:VAL:HG22	1:A:294:GLU:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLN:HB3	1:A:469:VAL:CG1	2.32	0.41
1:A:417:GLN:O	1:A:469:VAL:HG11	2.21	0.41
1:A:420:THR:N	1:A:421:PRO:CD	2.83	0.41
1:A:452:TYR:O	1:A:456:VAL:HG23	2.19	0.41
1:B:260:LEU:O	1:B:261:ALA:C	2.58	0.41
1:A:89:ASP:O	1:A:92:ALA:HB3	2.19	0.41
1:A:420:THR:CG2	1:A:527:THR:HG23	2.50	0.41
1:A:139:LEU:O	1:A:140:TYR:C	2.59	0.41
1:A:302:LEU:HA	1:A:303:PRO:HD2	1.84	0.41
1:A:165:PHE:CE2	1:A:182:LEU:HD21	2.56	0.41
1:A:114:ARG:NH1	1:A:520:GLU:OE2	2.50	0.41
1:A:22:LEU:CD2	1:A:151:ALA:HB1	2.50	0.41
1:B:268:GLN:HE21	1:B:268:GLN:HB2	1.65	0.41
1:B:394:LEU:HD12	1:B:394:LEU:HA	1.79	0.41
1:B:435:SER:O	1:B:439:LYS:HE2	2.20	0.41
1:B:307:ALA:O	1:B:312:SER:N	2.51	0.41
1:B:302:LEU:HA	1:B:303:PRO:HD2	1.83	0.41
1:A:36:PHE:CZ	1:A:136:LYS:HB3	2.55	0.41
1:A:250:LEU:N	1:A:250:LEU:HD23	2.36	0.41
1:A:81:ARG:C	1:A:83:THR:N	2.74	0.41
1:B:333:GLU:O	1:B:337:ARG:HG3	2.20	0.41
1:B:483:ASN:C	1:B:486:PRO:HD2	2.41	0.41
1:A:509:PHE:N	1:A:509:PHE:CD1	2.88	0.41
1:A:142:ILE:HD13	1:A:142:ILE:HA	1.78	0.41
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.47	0.40
1:A:424:VAL:HG21	1:A:527:THR:HA	2.02	0.40
1:A:524:LYS:HD3	1:A:524:LYS:HA	1.96	0.40
1:B:123:MET:HB3	1:B:165:PHE:HE2	1.85	0.40
1:B:566:THR:HB	1:B:567:CYS:H	1.76	0.40
1:A:411:TYR:O	1:A:414:LYS:HB3	2.21	0.40
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.35	0.40
1:B:543:GLN:HG3	1:B:544:LEU:N	2.36	0.40
1:A:441:PRO:C	1:A:443:ALA:N	2.75	0.40
1:B:416:PRO:O	1:B:534:LYS:HE2	2.21	0.40
1:B:264:ILE:HD12	1:B:290:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	576/585 (98%)	496 (86%)	60 (10%)	20 (4%)	4 6
1	B	576/585 (98%)	500 (87%)	65 (11%)	11 (2%)	10 16
All	All	1152/1170 (98%)	996 (86%)	125 (11%)	31 (3%)	6 9

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	GLU
1	B	60	GLU
1	B	501	GLU
1	B	538	LYS
1	B	566	THR
1	A	60	GLU
1	A	276	LYS
1	A	442	GLU
1	A	506	THR
1	A	566	THR
1	B	442	GLU
1	B	444	LYS
1	A	79	THR
1	B	59	ALA
1	A	17	GLU
1	A	59	ALA
1	A	283	LEU
1	A	321	GLU
1	A	480	SER
1	B	303	PRO
1	A	361	CYS
1	A	400	GLU
1	A	449	ALA
1	A	538	LYS
1	B	321	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	373	VAL
1	A	202	SER
1	A	466	LYS
1	A	537	PRO
1	B	85	GLY
1	A	493	VAL

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	506/511 (99%)	481 (95%)	25 (5%)	31 55
1	B	506/511 (99%)	473 (94%)	33 (6%)	21 39
All	All	1012/1022 (99%)	954 (94%)	58 (6%)	25 46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	96	PRO
1	A	109	ASN
1	A	111	ASN
1	A	149	PHE
1	A	183	ASP
1	A	187	ASP
1	A	208	GLU
1	A	232	SER
1	A	233	LYS
1	A	245	CYS
1	A	253	CYS
1	A	270	SER
1	A	276	LYS
1	A	375	ASP
1	A	479	GLU
1	A	489	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	506	THR
1	A	510	HIS
1	A	540	THR
1	A	548	MET
1	A	566	THR
1	A	567	CYS
1	A	568	PHE
1	A	580	GLN
1	B	30	TYR
1	B	34	CYS
1	B	58	SER
1	B	79	THR
1	B	83	THR
1	B	84	TYR
1	B	89	ASP
1	B	121	ASP
1	B	149	PHE
1	B	187	ASP
1	B	195	LYS
1	B	196	GLN
1	B	218	ARG
1	B	245	CYS
1	B	253	CYS
1	B	262	LYS
1	B	308	ASP
1	B	324	ASP
1	B	336	ARG
1	B	344	VAL
1	B	370	TYR
1	B	375	ASP
1	B	390	GLN
1	B	419	SER
1	B	427	SER
1	B	436	LYS
1	B	474	THR
1	B	479	GLU
1	B	515	THR
1	B	548	MET
1	B	566	THR
1	B	568	PHE
1	B	580	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	94	GLN
1	A	109	ASN
1	A	196	GLN
1	A	386	ASN
1	A	464	HIS
1	A	580	GLN
1	B	33	GLN
1	B	105	HIS
1	B	196	GLN
1	B	386	ASN
1	B	440	HIS
1	B	464	HIS
1	B	483	ASN
1	B	580	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.