Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:50 AM GMT

PDB ID	:	2BXE
Title	:	Human serum albumin complexed with diflunisal
Authors	:	Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on	:	2005-07-26
Resolution	:	2.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

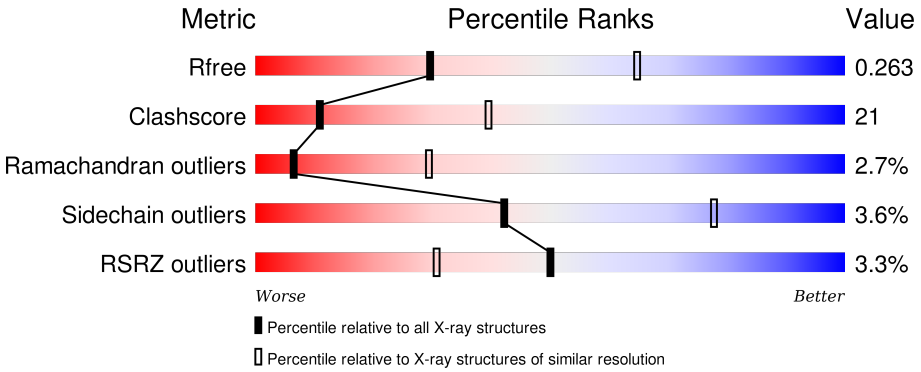
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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.

Mol	Chain	Length	Quality of chain
1	A	585	3% 61% 33%
1	B	585	4% 58% 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1FL	A	2003	-	-	-	X
2	1FL	B	2002	-	-	-	X
2	1FL	B	2003	-	-	-	X

2 Entry composition

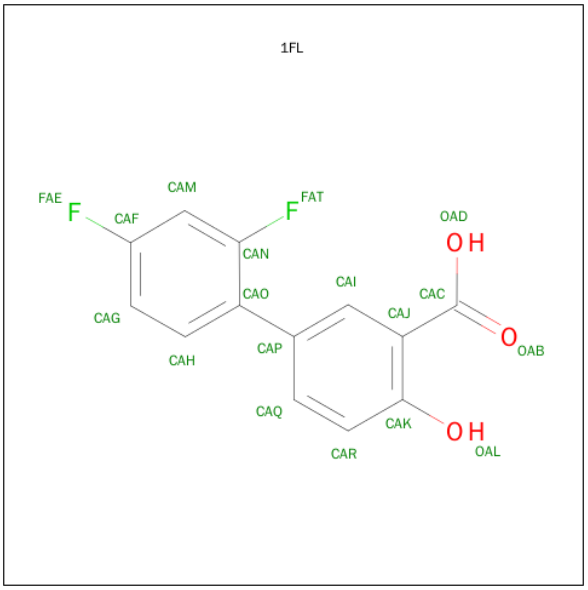
There are 2 unique types of molecules in this entry. The entry contains 8710 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	569	Total	C	N	O	S	0	0	0
			4344	2743	722	839	40			
1	B	566	Total	C	N	O	S	0	0	0
			4258	2692	710	816	40			

- Molecule 2 is 5-(2,4-DIFLUOROPHENYL)-2-HYDROXY-BENZOIC ACID (three-letter code: 1FL) (formula: $C_{13}H_8F_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		

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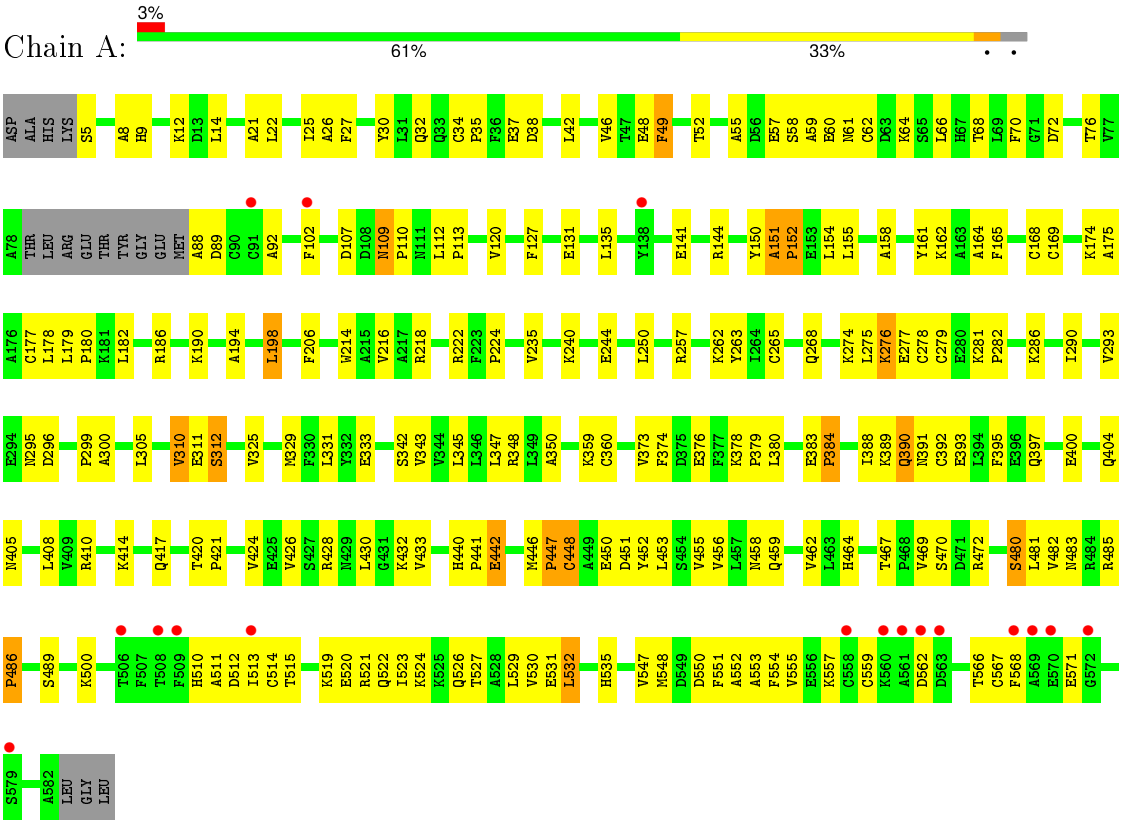
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		

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.

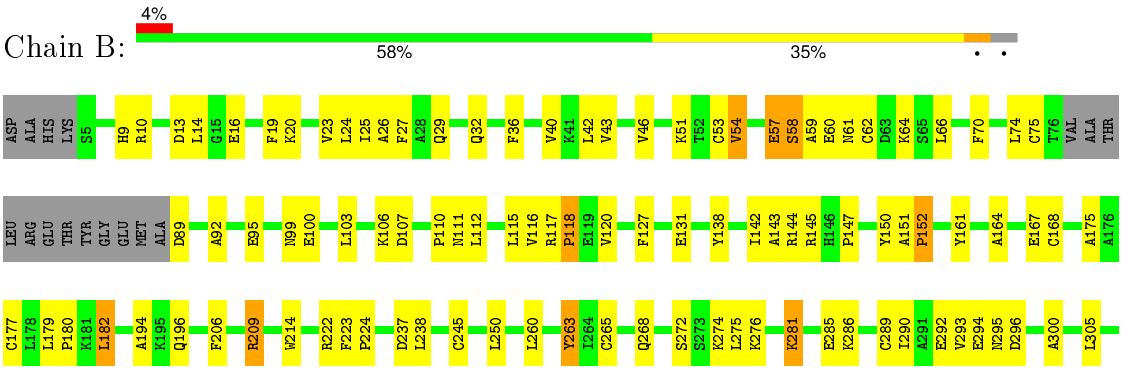
- Molecule 1: SERUM ALBUMIN

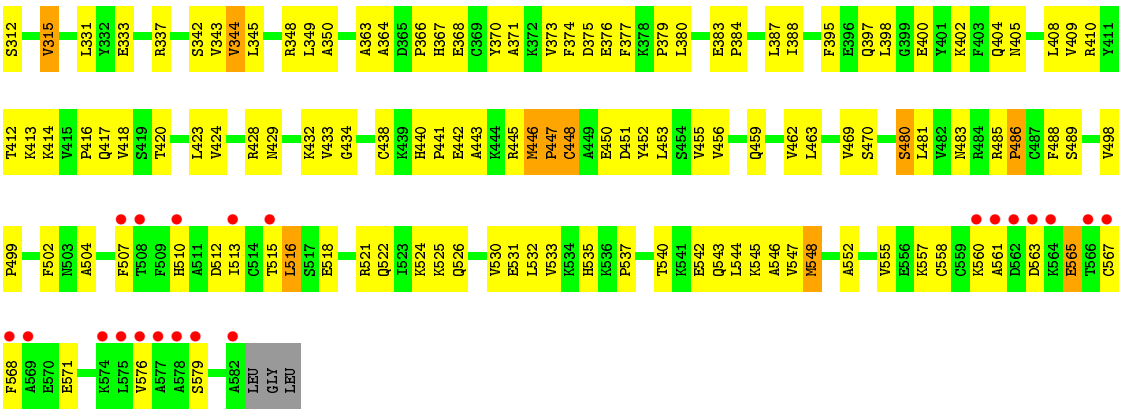
Chain A:



- Molecule 1: SERUM ALBUMIN

Chain B:




S312 V315 L331 Y332 E333 R337 S342 V343 V344 L345 R348 L349 A350 A363 A364 D365 P366 H367 E368 C369 Y370 A371 K372 V373 F374 D375 E376 F377 K378 P379 L380 E383 P384 L387 I388 F395 E396 Q397 L398 G399 E400 Y401 K402 F403 Q404 N405 L408 V409 R410 Y411
T412 K413 K414 V415 P416 Q417 V418 S419 T420 L423 V424 R428 N429 K432 V433 G434 C438 K439 H440 P441 E442 A443 K444 R445 M446 P447 C448 A449 E450 D451 Y452 L453 S454 V455 V456 Q459 V462 L463 V469 S470 S480 L481 V482 N483 R484 R485 P486 C487 F488 S489 V498
P499 F502 N503 A504 F507 T508 F509 H510 A511 D512 I513 C514 T515 L516 S517 E518 R521 Q522 I523 K524 K525 Q526 V530 E531 L532 V533 K534 H535 K536 P537 T540 K541 E542 Q543 L544 K545 A546 V547 M548 A552 V555 E556 K557 C558 C559 K560 A561 D562 D563 K564 E565 T566 C567
F568 A569 E570 E571 K574 L575 V576 A577 A578 S579 A582 LEU GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.41Å 55.53Å 120.52Å 81.54° 90.09° 65.93°	Depositor
Resolution (Å)	38.22 – 2.95 38.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.22-2.95) 92.8 (38.22-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.270 0.222 , 0.263	Depositor DCC
R_{free} test set	1296 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 27267 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8710	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1FL

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	0.45	0/4428	0.66	0/6011
1	B	0.45	0/4339	0.65	0/5895
All	All	0.45	0/8767	0.65	0/11906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4344	0	4056	159	0
1	B	4258	0	3962	193	0
2	A	54	0	18	3	0
2	B	54	0	18	7	0
All	All	8710	0	8054	352	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 (352) 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:433:VAL:HG22	1:A:452:TYR:HD2	1.06	1.10
1:A:433:VAL:HG22	1:A:452:TYR:CD2	1.91	1.05
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.30	0.95
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.02	0.93
1:B:222:ARG:HD3	2:B:2003:1FL:FAE	1.59	0.91
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.53	0.88
1:A:222:ARG:HD3	2:A:2003:1FL:FAE	1.63	0.88
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.55	0.87
1:B:364:ALA:O	1:B:366:PRO:HD3	1.75	0.87
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.74	0.85
1:B:57:GLU:HG3	1:B:58:SER:H	1.42	0.85
1:B:567:CYS:SG	1:B:571:GLU:HB2	2.16	0.85
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.56	0.85
1:A:276:LYS:HD2	1:A:277:GLU:H	1.42	0.83
1:A:222:ARG:HG3	1:A:295:ASN:OD1	1.79	0.82
1:B:540:THR:HG23	1:B:543:GLN:H	1.42	0.81
1:A:120:VAL:HG11	1:A:174:LYS:HB2	1.61	0.81
1:B:222:ARG:HG3	1:B:295:ASN:OD1	1.79	0.81
1:A:417:GLN:OE1	1:A:417:GLN:N	2.13	0.80
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.60	0.80
1:A:424:VAL:O	1:A:428:ARG:HG3	1.82	0.80
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.64	0.79
1:A:390:GLN:O	1:A:393:GLU:N	2.13	0.79
1:B:281:LYS:HD2	1:B:285:GLU:HG2	1.65	0.79
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.66	0.78
1:A:550:ASP:O	1:A:554:PHE:HD1	1.66	0.78
1:A:182:LEU:O	1:A:186:ARG:HG2	1.84	0.78
1:A:547:VAL:HG12	1:A:551:PHE:HE1	1.46	0.77
1:B:345:LEU:HD22	1:B:446:MET:CE	2.15	0.77
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.50	0.77
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.69	0.75
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.27	0.74
1:A:107:ASP:OD2	1:A:110:PRO:HA	1.87	0.74
1:B:265:CYS:O	1:B:268:GLN:HG3	1.88	0.74
1:A:547:VAL:CG1	1:A:551:PHE:HE1	2.00	0.74
1:B:110:PRO:HB2	1:B:112:LEU:CD2	2.17	0.74
1:A:169:CYS:HA	1:A:174:LYS:HD3	1.71	0.73
1:A:414:LYS:O	1:A:472:ARG:NH1	2.23	0.72
1:B:127:PHE:O	1:B:131:GLU:HB3	1.91	0.71
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.71	0.71
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.73	0.70
1:A:376:GLU:O	1:A:379:PRO:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.55	0.70
1:B:499:PRO:HB3	1:B:535:HIS:O	1.89	0.70
1:A:400:GLU:O	1:A:404:GLN:HG3	1.91	0.70
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.75	0.69
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.22	0.69
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.27	0.69
1:B:285:GLU:O	1:B:289:CYS:HB2	1.93	0.69
1:B:561:ALA:HB3	1:B:563:ASP:OD1	1.93	0.69
1:B:483:ASN:O	1:B:486:PRO:HD2	1.92	0.68
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.29	0.68
1:A:276:LYS:CD	1:A:277:GLU:H	2.06	0.68
1:B:510:HIS:HA	1:B:568:PHE:CD2	2.28	0.68
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.24	0.68
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.76	0.68
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.25	0.67
1:B:260:LEU:O	1:B:260:LEU:HD23	1.94	0.67
1:B:32:GLN:NE2	1:B:110:PRO:HG2	2.10	0.67
1:A:35:PRO:HD2	1:A:38:ASP:OD2	1.95	0.67
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.77	0.66
1:B:110:PRO:HB2	1:B:112:LEU:HD22	1.76	0.66
1:B:10:ARG:O	1:B:14:LEU:HD23	1.95	0.66
1:B:344:VAL:HG22	1:B:451:ASP:OD1	1.96	0.65
1:B:565:GLU:O	1:B:568:PHE:HB3	1.96	0.65
1:A:66:LEU:O	1:A:70:PHE:HD1	1.78	0.65
1:B:290:ILE:O	1:B:293:VAL:HG12	1.98	0.64
1:A:483:ASN:O	1:A:486:PRO:HD2	1.98	0.64
1:A:276:LYS:HD3	1:A:277:GLU:HG2	1.81	0.63
1:A:529:LEU:HD22	1:A:548:MET:CE	2.28	0.63
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.33	0.63
1:B:66:LEU:O	1:B:70:PHE:HD1	1.82	0.63
1:B:400:GLU:O	1:B:404:GLN:HG3	1.97	0.62
1:B:441:PRO:O	1:B:443:ALA:N	2.31	0.62
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.28	0.62
1:A:198:LEU:HD22	1:A:455:VAL:HA	1.82	0.61
1:B:558:CYS:SG	1:B:571:GLU:HB3	2.40	0.61
1:A:240:LYS:O	1:A:244:GLU:HG3	2.01	0.61
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.82	0.61
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.54	0.60
1:B:116:VAL:O	1:B:118:PRO:HD3	2.01	0.60
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.83	0.60
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LYS:O	1:A:523:ILE:HG13	2.02	0.60
1:B:42:LEU:O	1:B:46:VAL:HG23	2.02	0.59
1:A:150:TYR:OH	2:A:2003:1FL:OAD	2.19	0.59
1:B:263:TYR:C	1:B:263:TYR:CD2	2.75	0.59
1:A:426:VAL:O	1:A:430:LEU:HG	2.03	0.59
1:B:441:PRO:C	1:B:443:ALA:H	2.04	0.59
1:B:32:GLN:HE22	1:B:110:PRO:CG	2.16	0.59
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.85	0.59
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.38	0.58
1:B:29:GLN:HG2	1:B:143:ALA:O	2.03	0.58
1:B:510:HIS:HA	1:B:568:PHE:HD2	1.66	0.58
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.31	0.58
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.86	0.58
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.58
1:B:513:ILE:HD12	1:B:555:VAL:HG23	1.85	0.57
1:A:450:GLU:HG3	1:A:450:GLU:O	2.03	0.57
1:B:417:GLN:H	1:B:417:GLN:CD	2.07	0.57
1:B:424:VAL:O	1:B:428:ARG:HG3	2.04	0.57
1:B:518:GLU:O	1:B:522:GLN:HG3	2.04	0.57
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.87	0.57
1:A:510:HIS:HA	1:A:568:PHE:CB	2.35	0.57
1:B:532:LEU:HD21	1:B:547:VAL:HG11	1.87	0.57
1:B:27:PHE:CD2	1:B:74:LEU:HD21	2.40	0.56
1:B:32:GLN:NE2	1:B:110:PRO:CG	2.67	0.56
1:B:424:VAL:HG23	1:B:530:VAL:HG21	1.86	0.56
1:B:117:ARG:NH2	1:B:182:LEU:HB3	2.19	0.56
1:A:345:LEU:HD23	1:A:446:MET:CE	2.35	0.56
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.36	0.56
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.30	0.56
1:B:405:ASN:O	1:B:409:VAL:HG23	2.04	0.56
1:A:5:SER:HA	1:A:62:CYS:O	2.05	0.56
1:B:502:PHE:HE2	1:B:507:PHE:HB2	1.70	0.56
1:B:376:GLU:O	1:B:379:PRO:HD2	2.06	0.56
1:B:543:GLN:O	1:B:546:ALA:HB3	2.06	0.55
1:B:513:ILE:CD1	1:B:555:VAL:HG23	2.36	0.55
1:B:107:ASP:HB3	1:B:110:PRO:HG3	1.87	0.55
1:B:260:LEU:HD22	2:B:2003:1FL:HAR	1.87	0.55
1:B:441:PRO:C	1:B:443:ALA:N	2.58	0.55
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.89	0.55
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.35	0.55
1:B:168:CYS:SG	1:B:177:CYS:C	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:MET:CB	1:B:447:PRO:HD3	2.37	0.55
1:A:325:VAL:O	1:A:329:MET:HG3	2.07	0.55
1:B:558:CYS:SG	1:B:571:GLU:CB	2.95	0.54
1:A:550:ASP:O	1:A:554:PHE:CD1	2.55	0.54
1:A:8:ALA:O	1:A:12:LYS:HG2	2.07	0.54
1:B:502:PHE:CE2	1:B:507:PHE:HB2	2.42	0.54
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.90	0.54
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.90	0.54
1:B:57:GLU:O	1:B:58:SER:C	2.46	0.54
1:A:380:LEU:O	1:A:384:PRO:HD2	2.08	0.53
1:A:222:ARG:C	1:A:224:PRO:HD3	2.29	0.53
1:A:547:VAL:CG1	1:A:551:PHE:CE1	2.88	0.53
1:B:117:ARG:HH22	1:B:182:LEU:HB3	1.73	0.53
1:A:276:LYS:CD	1:A:277:GLU:HG2	2.38	0.53
1:B:345:LEU:HD22	1:B:446:MET:HE1	1.89	0.53
1:A:89:ASP:O	1:A:92:ALA:HB3	2.09	0.53
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.90	0.53
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.91	0.53
1:A:522:GLN:O	1:A:526:GLN:HG3	2.09	0.53
1:B:567:CYS:SG	1:B:571:GLU:CB	2.95	0.53
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.90	0.52
1:B:516:LEU:H	1:B:516:LEU:HD12	1.74	0.52
1:B:115:LEU:HG	1:B:145:ARG:CZ	2.39	0.52
1:B:32:GLN:HE22	1:B:110:PRO:HG3	1.74	0.52
1:B:480:SER:OG	1:B:483:ASN:HB2	2.09	0.52
1:B:440:HIS:HB3	1:B:441:PRO:CD	2.39	0.52
1:A:279:CYS:HA	1:A:286:LYS:CD	2.40	0.52
1:A:49:PHE:O	1:A:49:PHE:HD2	1.93	0.52
1:A:464:HIS:HE1	1:A:470:SER:H	1.58	0.52
1:B:540:THR:HG22	1:B:543:GLN:HB2	1.91	0.52
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.92	0.51
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.36	0.51
1:A:480:SER:OG	1:A:483:ASN:HB2	2.10	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.10	0.51
1:A:342:SER:HB2	1:A:451:ASP:OD2	2.10	0.51
1:A:161:TYR:O	1:A:164:ALA:HB3	2.11	0.51
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.92	0.51
1:B:432:LYS:O	1:B:433:VAL:C	2.47	0.51
1:A:9:HIS:C	1:A:9:HIS:HD1	2.14	0.51
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.40	0.51
1:B:237:ASP:CB	1:B:260:LEU:HD12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:LYS:HA	1:B:54:VAL:HG23	1.92	0.50
1:B:418:VAL:CG1	1:B:423:LEU:HG	2.41	0.50
1:B:408:LEU:O	1:B:412:THR:OG1	2.20	0.50
1:A:531:GLU:HA	1:A:531:GLU:OE1	2.12	0.50
1:A:464:HIS:CE1	1:A:469:VAL:H	2.30	0.50
1:A:343:VAL:O	1:A:347:LEU:HG	2.12	0.50
1:B:456:VAL:O	1:B:459:GLN:N	2.42	0.50
1:B:535:HIS:O	1:B:537:PRO:HD3	2.11	0.50
1:B:36:PHE:O	1:B:40:VAL:HG23	2.11	0.50
1:A:420:THR:O	1:A:424:VAL:HG23	2.11	0.50
1:B:409:VAL:O	1:B:413:LYS:HG3	2.12	0.49
1:B:150:TYR:HB2	1:B:196:GLN:HG2	1.94	0.49
1:A:345:LEU:HD23	1:A:446:MET:HE1	1.94	0.49
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.49
1:A:186:ARG:O	1:A:190:LYS:HG3	2.12	0.49
1:B:535:HIS:C	1:B:537:PRO:HD3	2.31	0.49
1:B:384:PRO:O	1:B:388:ILE:HG12	2.13	0.49
1:A:447:PRO:O	1:A:448:CYS:C	2.50	0.49
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.76	0.49
1:A:42:LEU:O	1:A:46:VAL:HG23	2.12	0.49
1:B:100:GLU:HG2	1:B:103:LEU:HD12	1.93	0.49
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.13	0.49
1:A:417:GLN:CD	1:A:417:GLN:H	2.08	0.49
1:A:49:PHE:O	1:A:49:PHE:CD2	2.66	0.49
1:B:552:ALA:O	1:B:555:VAL:HG12	2.13	0.49
1:A:551:PHE:O	1:A:552:ALA:C	2.50	0.48
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.95	0.48
1:A:512:ASP:O	1:A:515:THR:HG22	2.14	0.48
1:A:155:LEU:O	1:A:158:ALA:HB3	2.13	0.48
1:B:417:GLN:N	1:B:417:GLN:CD	2.66	0.48
1:B:576:VAL:HA	1:B:579:SER:HB2	1.94	0.48
1:B:66:LEU:O	1:B:70:PHE:CD1	2.64	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.96	0.48
1:A:342:SER:HB3	1:A:447:PRO:HA	1.94	0.48
1:B:481:LEU:N	2:B:2002:1FL:OAB	2.42	0.48
1:B:498:VAL:O	1:B:498:VAL:HG23	2.14	0.48
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.48	0.48
1:A:388:ILE:O	1:A:389:LYS:C	2.52	0.48
1:B:453:LEU:HD22	2:B:2001:1FL:HAQ	1.96	0.48
1:A:27:PHE:CE2	1:A:70:PHE:HD2	2.32	0.47
1:B:237:ASP:HB3	1:B:260:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:SER:HB3	1:B:447:PRO:HA	1.95	0.47
1:B:483:ASN:O	1:B:486:PRO:CD	2.62	0.47
1:B:274:LYS:CE	1:B:296:ASP:HA	2.44	0.47
1:A:275:LEU:HD23	1:A:293:VAL:HG11	1.96	0.47
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.96	0.47
1:A:66:LEU:O	1:A:70:PHE:CD1	2.65	0.47
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.14	0.47
1:A:168:CYS:SG	1:A:177:CYS:C	2.93	0.47
1:A:218:ARG:HD3	1:A:343:VAL:HG21	1.97	0.47
1:B:542:GLU:OE1	1:B:542:GLU:HA	2.14	0.47
1:A:550:ASP:O	1:A:553:ALA:HB3	2.15	0.47
1:B:453:LEU:CD2	2:B:2001:1FL:HAQ	2.44	0.47
1:B:260:LEU:C	1:B:260:LEU:HD23	2.35	0.47
1:B:540:THR:HG22	1:B:543:GLN:CG	2.45	0.47
1:B:9:HIS:HD2	1:B:13:ASP:OD2	1.96	0.47
1:A:532:LEU:O	1:A:535:HIS:HB3	2.15	0.47
1:A:32:GLN:HG2	1:A:144:ARG:O	2.15	0.47
1:B:521:ARG:O	1:B:525:LYS:HG3	2.15	0.46
1:B:384:PRO:HB2	1:B:446:MET:SD	2.55	0.46
1:A:88:ALA:O	1:A:89:ASP:C	2.53	0.46
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.96	0.46
1:B:151:ALA:CB	1:B:152:PRO:CD	2.93	0.46
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.96	0.46
1:B:138:TYR:O	1:B:142:ILE:HG12	2.14	0.46
1:A:390:GLN:O	1:A:392:CYS:N	2.49	0.46
1:A:206:PHE:CZ	1:A:481:LEU:HB2	2.51	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.97	0.46
1:B:312:SER:O	1:B:315:VAL:HG23	2.16	0.46
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.51	0.45
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.51	0.45
1:A:265:CYS:O	1:A:268:GLN:HG3	2.15	0.45
1:B:522:GLN:HA	1:B:525:LYS:HD3	1.98	0.45
1:A:555:VAL:O	1:A:559:CYS:HB2	2.16	0.45
1:B:462:VAL:HG23	1:B:463:LEU:N	2.32	0.45
1:A:206:PHE:CE2	1:A:481:LEU:HB2	2.50	0.45
1:B:292:GLU:HG2	1:B:292:GLU:O	2.17	0.45
1:A:61:ASN:ND2	1:A:64:LYS:HE3	2.27	0.45
1:B:521:ARG:O	1:B:524:LYS:HB2	2.16	0.45
1:A:420:THR:CG2	1:A:527:THR:HG23	2.47	0.45
1:A:456:VAL:O	1:A:459:GLN:N	2.50	0.45
1:A:21:ALA:HB1	1:A:155:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ASN:O	1:B:432:LYS:HB2	2.17	0.45
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.46	0.45
1:B:485:ARG:HE	1:B:485:ARG:HB3	1.63	0.45
1:A:66:LEU:HD22	1:A:70:PHE:HE1	1.82	0.45
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.99	0.45
1:A:520:GLU:O	1:A:524:LYS:HG3	2.17	0.45
1:B:19:PHE:O	1:B:23:VAL:HG23	2.17	0.45
1:B:150:TYR:OH	2:B:2003:1FL:OAB	2.22	0.44
1:A:500:LYS:O	1:A:535:HIS:ND1	2.47	0.44
1:A:532:LEU:HD11	1:A:547:VAL:HG11	1.99	0.44
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.44
1:A:290:ILE:HA	1:A:293:VAL:HG13	1.99	0.44
1:A:511:ALA:O	1:A:514:CYS:SG	2.76	0.44
1:B:274:LYS:HE2	1:B:296:ASP:HA	1.98	0.44
1:A:405:ASN:O	1:A:408:LEU:HB2	2.17	0.44
1:B:533:VAL:CG2	1:B:544:LEU:HD21	2.48	0.44
1:B:558:CYS:C	1:B:560:LYS:H	2.20	0.44
1:B:16:GLU:O	1:B:20:LYS:HG3	2.18	0.44
1:A:521:ARG:O	1:A:524:LYS:N	2.48	0.44
1:B:274:LYS:HD2	1:B:294:GLU:OE2	2.18	0.44
1:A:441:PRO:O	1:A:442:GLU:C	2.56	0.44
1:A:30:TYR:CD1	1:A:102:PHE:HB3	2.53	0.44
1:B:14:LEU:N	1:B:14:LEU:HD22	2.33	0.44
1:B:286:LYS:O	1:B:289:CYS:HB3	2.18	0.44
1:A:216:VAL:HG22	1:A:235:VAL:HG21	2.00	0.44
1:A:278:CYS:O	1:A:281:LYS:HG2	2.18	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.88	0.43
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.41	0.43
1:B:502:PHE:CZ	1:B:504:ALA:HA	2.54	0.43
1:A:567:CYS:O	1:A:571:GLU:N	2.46	0.43
1:B:483:ASN:C	1:B:486:PRO:HD2	2.38	0.43
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.17	0.43
1:A:257:ARG:HG2	1:A:257:ARG:O	2.18	0.43
1:B:161:TYR:O	1:B:164:ALA:HB3	2.17	0.43
1:A:458:ASN:O	1:A:462:VAL:HG22	2.18	0.43
1:B:567:CYS:O	1:B:571:GLU:N	2.50	0.43
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.45	0.43
1:B:533:VAL:HG22	1:B:544:LEU:HD21	2.01	0.43
1:B:557:LYS:HB3	1:B:571:GLU:OE2	2.18	0.43
1:B:558:CYS:C	1:B:560:LYS:N	2.71	0.43
1:B:110:PRO:HB2	1:B:112:LEU:HD21	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:O	1:A:72:ASP:OD2	2.37	0.43
1:B:414:LYS:HE3	1:B:488:PHE:O	2.19	0.43
1:B:433:VAL:O	1:B:434:GLY:C	2.54	0.43
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.54	0.43
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.91	0.43
1:B:194:ALA:HB1	1:B:455:VAL:HG13	2.01	0.42
1:B:209:ARG:HH21	2:B:2002:1FL:HAH	1.84	0.42
1:B:447:PRO:O	1:B:448:CYS:C	2.57	0.42
1:B:410:ARG:O	1:B:414:LYS:HG3	2.20	0.42
1:B:417:GLN:OE1	1:B:417:GLN:N	2.35	0.42
1:B:333:GLU:O	1:B:337:ARG:HG3	2.19	0.42
1:B:51:LYS:C	1:B:53:CYS:H	2.23	0.42
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.42
1:B:531:GLU:OE1	1:B:531:GLU:HA	2.19	0.42
1:A:483:ASN:O	1:A:486:PRO:CD	2.64	0.42
1:A:432:LYS:O	1:A:433:VAL:C	2.56	0.42
1:B:89:ASP:O	1:B:92:ALA:HB3	2.18	0.42
1:B:434:GLY:HA2	1:B:438:CYS:SG	2.60	0.42
1:A:345:LEU:HD23	1:A:446:MET:HE3	2.02	0.42
1:A:48:GLU:O	1:A:52:THR:HG23	2.20	0.42
1:A:25:ILE:HD13	1:A:154:LEU:HD23	2.01	0.42
1:B:563:ASP:OD2	1:B:567:CYS:N	2.50	0.41
1:B:107:ASP:O	1:B:110:PRO:HG3	2.20	0.41
1:A:464:HIS:CE1	1:A:470:SER:H	2.36	0.41
1:B:367:HIS:O	1:B:371:ALA:HB2	2.19	0.41
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.62	0.41
1:B:540:THR:CG2	1:B:543:GLN:HB2	2.50	0.41
1:A:384:PRO:HB2	1:A:446:MET:SD	2.60	0.41
1:B:293:VAL:HG22	1:B:294:GLU:N	2.34	0.41
1:B:512:ASP:O	1:B:515:THR:HG22	2.21	0.41
1:B:117:ARG:HG3	1:B:117:ARG:O	2.21	0.41
1:B:545:LYS:HA	1:B:548:MET:HB2	2.01	0.41
1:B:540:THR:CG2	1:B:543:GLN:HG3	2.51	0.41
1:A:120:VAL:CG1	1:A:174:LYS:HB2	2.41	0.41
1:A:373:VAL:O	1:A:376:GLU:HB2	2.21	0.41
1:A:290:ILE:O	1:A:293:VAL:HG22	2.21	0.41
1:B:107:ASP:OD2	1:B:110:PRO:HA	2.20	0.41
1:B:417:GLN:HB2	1:B:470:SER:HB2	2.03	0.41
1:B:349:LEU:HD22	1:B:377:PHE:CG	2.55	0.41
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.01	0.41
1:A:395:PHE:O	1:A:397:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASP:HB2	1:B:260:LEU:HD12	2.02	0.41
1:A:274:LYS:HA	1:A:276:LYS:HE3	2.02	0.41
1:B:32:GLN:NE2	1:B:144:ARG:O	2.45	0.41
1:B:412:THR:O	1:B:416:PRO:HG3	2.21	0.41
1:A:158:ALA:O	1:A:161:TYR:HB3	2.21	0.41
1:B:459:GLN:O	1:B:462:VAL:HG22	2.21	0.41
1:B:395:PHE:C	1:B:397:GLN:N	2.74	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.87	0.41
1:A:453:LEU:CD2	2:A:2001:1FL:HAQ	2.51	0.41
1:A:262:LYS:O	1:A:263:TYR:C	2.59	0.41
1:A:310:VAL:HG11	1:A:374:PHE:CE1	2.56	0.40
1:B:441:PRO:O	1:B:445:ARG:HG3	2.21	0.40
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.51	0.40
1:B:370:TYR:C	1:B:370:TYR:CD1	2.95	0.40
1:B:380:LEU:O	1:B:384:PRO:CD	2.68	0.40
1:A:410:ARG:O	1:A:414:LYS:HG3	2.22	0.40
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.40
1:B:61:ASN:HD22	1:B:64:LYS:CD	2.35	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40
1:A:359:LYS:HG3	1:A:360:CYS:N	2.36	0.40
1:B:446:MET:CB	1:B:447:PRO:CD	2.99	0.40
1:A:408:LEU:HD22	1:A:530:VAL:HG22	2.03	0.40
1:A:566:THR:C	1:A:568:PHE:N	2.73	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	565/585 (97%)	486 (86%)	65 (12%)	14 (2%)	7 31
1	B	562/585 (96%)	478 (85%)	68 (12%)	16 (3%)	6 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1127/1170 (96%)	964 (86%)	133 (12%)	30 (3%)	6 29

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	60	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	300	ALA
1	B	565	GLU
1	A	390	GLN
1	A	391	ASN
1	A	562	ASP
1	B	442	GLU
1	A	58	SER
1	A	312	SER
1	A	447	PRO
1	A	557	LYS
1	B	315	VAL
1	B	363	ALA
1	A	300	ALA
1	A	448	CYS
1	B	447	PRO
1	A	57	GLU
1	B	276	LYS
1	A	55	ALA
1	B	60	GLU
1	B	75	CYS
1	B	281	LYS
1	B	448	CYS
1	B	118	PRO
1	B	469	VAL
1	A	151	ALA

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	447/511 (88%)	432 (97%)	15 (3%)	44 79
1	B	432/511 (84%)	415 (96%)	17 (4%)	39 75
All	All	879/1022 (86%)	847 (96%)	32 (4%)	42 78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	49	PHE
1	A	109	ASN
1	A	152	PRO
1	A	198	LEU
1	A	276	LYS
1	A	310	VAL
1	A	384	PRO
1	A	440	HIS
1	A	442	GLU
1	A	467	THR
1	A	480	SER
1	A	486	PRO
1	A	489	SER
1	A	532	LEU
1	B	111	ASN
1	B	152	PRO
1	B	167	GLU
1	B	182	LEU
1	B	209	ARG
1	B	245	CYS
1	B	263	TYR
1	B	344	VAL
1	B	368	GLU
1	B	375	ASP
1	B	387	LEU
1	B	446	MET
1	B	480	SER
1	B	486	PRO
1	B	489	SER
1	B	516	LEU
1	B	548	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	318	ASN
1	A	338	HIS
1	A	429	ASN
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
1	B	9	HIS
1	B	111	ASN
1	B	338	HIS
1	B	464	HIS
1	B	483	ASN

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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	1FL	A	2001	-	16,19,19	1.39	2 (12%)	23,27,27	1.13	1 (4%)
2	1FL	A	2002	-	16,19,19	1.34	1 (6%)	23,27,27	1.20	3 (13%)
2	1FL	A	2003	-	16,19,19	0.54	0	23,27,27	1.00	0
2	1FL	B	2001	-	16,19,19	1.41	1 (6%)	23,27,27	1.10	1 (4%)
2	1FL	B	2002	-	16,19,19	1.36	1 (6%)	23,27,27	1.23	3 (13%)
2	1FL	B	2003	-	16,19,19	1.34	2 (12%)	23,27,27	1.34	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1FL	A	2001	-	-	0/4/8/8	0/2/2/2
2	1FL	A	2002	-	-	0/4/8/8	0/2/2/2
2	1FL	A	2003	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2001	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2002	-	-	0/4/8/8	0/2/2/2
2	1FL	B	2003	-	-	0/4/8/8	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	1FL	CAM-CAN	2.10	1.41	1.37
2	B	2003	1FL	CAH-CAG	2.30	1.42	1.38
2	B	2003	1FL	CAH-CAO	3.12	1.45	1.39
2	B	2002	1FL	CAO-CAN	3.59	1.43	1.38
2	A	2001	1FL	CAO-CAN	3.60	1.43	1.38
2	A	2002	1FL	CAO-CAN	3.64	1.43	1.38
2	B	2001	1FL	CAO-CAN	3.73	1.43	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2003	1FL	CAH-CAG-CAF	-2.28	115.88	118.35
2	A	2002	1FL	FAT-CAN-CAM	-2.07	114.70	118.59
2	B	2002	1FL	FAT-CAN-CAM	-2.02	114.80	118.59
2	A	2002	1FL	CAN-CAM-CAF	2.02	118.74	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2003	1FL	OAL-CAK-CAJ	2.07	125.70	120.02
2	B	2002	1FL	CAN-CAM-CAF	2.15	118.87	116.63
2	A	2001	1FL	FAT-CAN-CAO	2.23	122.12	118.80
2	B	2001	1FL	FAT-CAN-CAO	2.31	122.23	118.80
2	B	2003	1FL	CAN-CAM-CAF	2.88	119.64	116.63
2	B	2002	1FL	FAT-CAN-CAO	2.99	123.24	118.80
2	A	2002	1FL	FAT-CAN-CAO	3.01	123.28	118.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	1FL	1	0
2	A	2003	1FL	2	0
2	B	2001	1FL	2	0
2	B	2002	1FL	2	0
2	B	2003	1FL	3	0

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, 95^{th} 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	569/585 (97%)	-0.17	17 (2%)	54	33	35, 78, 156, 170	0
1	B	566/585 (96%)	-0.07	21 (3%)	45	27	35, 78, 148, 175	0
All	All	1135/1170 (97%)	-0.12	38 (3%)	50	31	35, 78, 150, 175	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	ALA	6.4
1	B	566	THR	6.3
1	B	562	ASP	5.8
1	B	579	SER	5.7
1	B	575	LEU	5.6
1	B	577	ALA	5.4
1	B	564	LYS	4.9
1	A	508	THR	4.8
1	B	578	ALA	4.7
1	B	508	THR	4.4
1	A	563	ASP	3.7
1	B	568	PHE	3.5
1	B	561	ALA	3.1
1	B	513	ILE	2.9
1	A	569	ALA	2.8
1	A	572	GLY	2.8
1	A	579	SER	2.7
1	B	563	ASP	2.7
1	A	506	THR	2.7
1	B	507	PHE	2.7
1	A	560	LYS	2.7
1	A	570	GLU	2.6
1	B	576	VAL	2.5
1	A	513	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	574	LYS	2.5
1	A	561	ALA	2.5
1	A	91	CYS	2.4
1	A	138	TYR	2.3
1	A	558	CYS	2.3
1	A	562	ASP	2.3
1	B	560	LYS	2.3
1	B	569	ALA	2.2
1	B	510	HIS	2.2
1	B	567	CYS	2.1
1	A	102	PHE	2.1
1	B	515	THR	2.1
1	A	568	PHE	2.0
1	A	509	PHE	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	1FL	B	2003	18/18	0.87	0.36	4.14	98,101,102,104	0
2	1FL	A	2003	18/18	0.84	0.28	3.32	109,109,111,111	0
2	1FL	B	2002	18/18	0.92	0.31	2.85	91,94,99,100	0
2	1FL	B	2001	18/18	0.93	0.25	1.91	63,67,71,73	0
2	1FL	A	2002	18/18	0.91	0.24	1.46	77,82,91,92	0
2	1FL	A	2001	18/18	0.95	0.20	0.64	55,58,66,68	0

6.5 Other polymers (i)

There are no such residues in this entry.