Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 02:03 pm GMT

PDB ID	:	2BXG
Title	:	Human serum albumin complexed with ibuprofen
Authors	:	Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on	:	2005-07-26
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

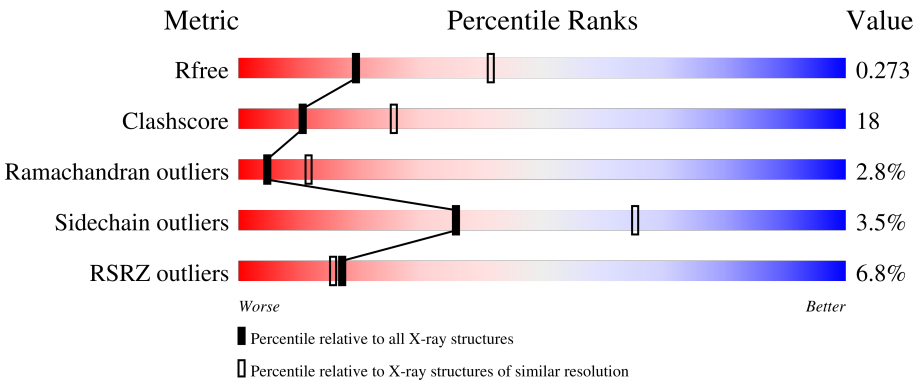
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 >=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 <=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	6% 66% 30% • •
1	B	585	7% 59% 37% • •

2 Entry composition (i)

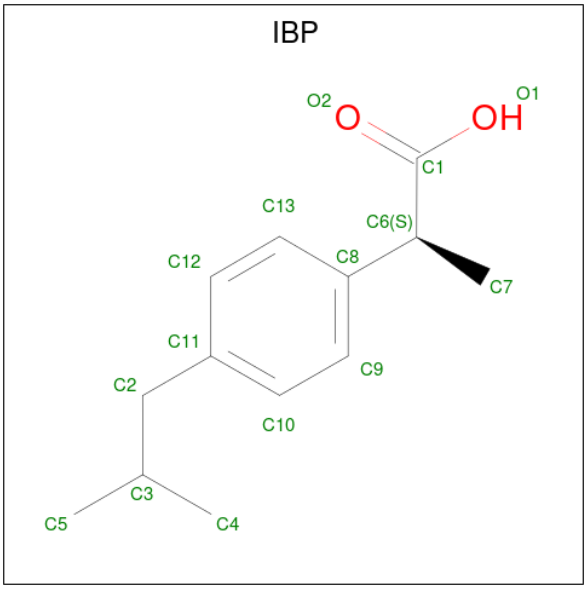
There are 2 unique types of molecules in this entry. The entry contains 8773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	578	4360	2743	738	839	40	0	0	0
1	B	578	4353	2739	730	843	41	0	0	0

- Molecule 2 is IBUPROFEN (three-letter code: IBP) (formula: $C_{13}H_{18}O_2$).



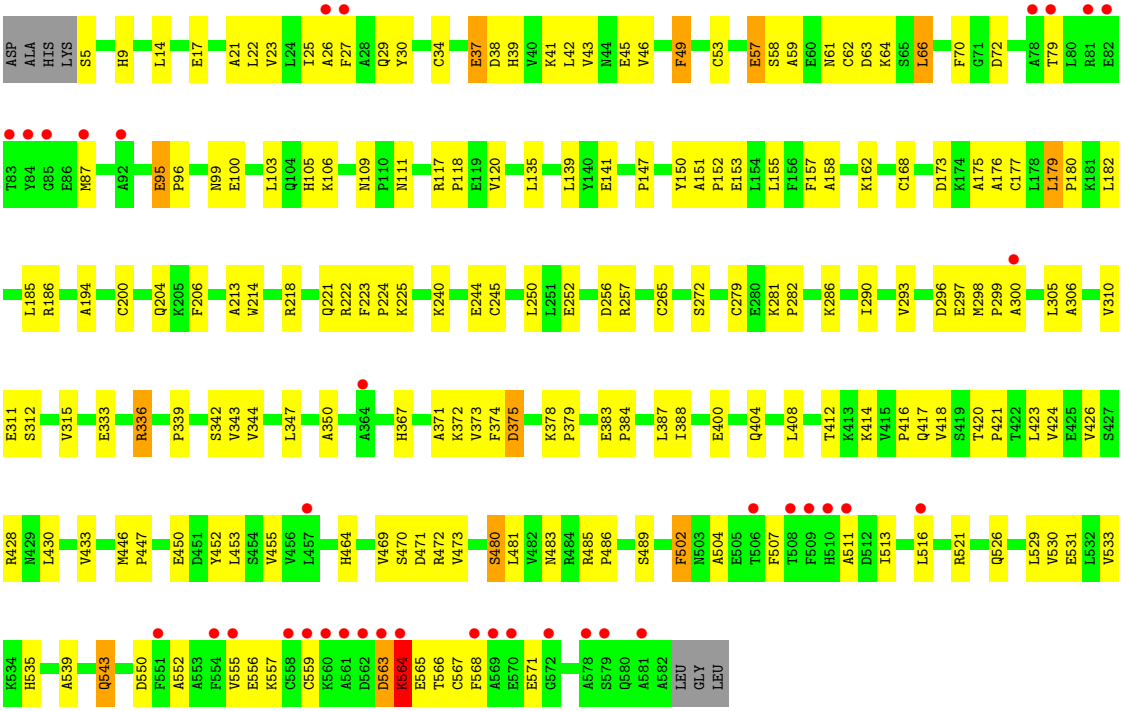
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	15	13	2	0	0
2	A	1	15	13	2	0	0
2	B	1	15	13	2	0	0
2	B	1	15	13	2	0	0

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 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.

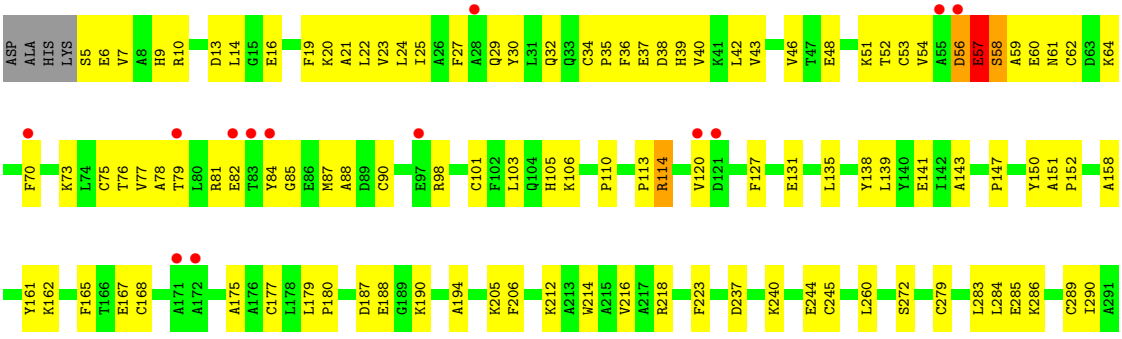
• Molecule 1: SERUM ALBUMIN

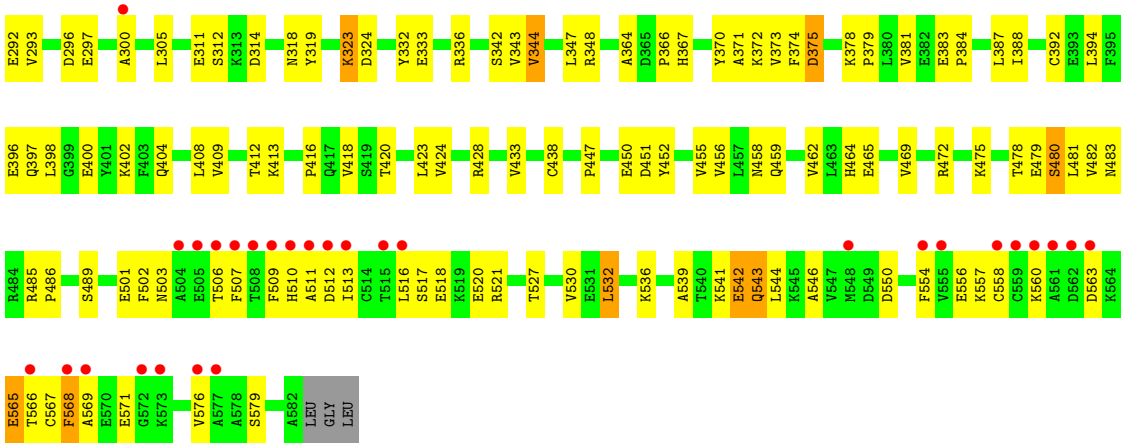
Chain A:



• Molecule 1: SERUM ALBUMIN

Chain B:




E565 T566 C567 F568 A569 E570 E571 G572 K573 V576 A577 A578 S579 A582 LEU GLY LEU
R484 R485 P486 S489 E501 F502 N503 A504 E505 T506 F507 T508 F509 H510 A511 D512 I513 C514 T515 L516 S517 E518 K519 E520 R521 T527 V530 E531 L532 K536 A539 T540 K541 E542 Q543 L544 K545 A546 V547 M548 D549 D550 F554 V555 E556 K557 C558 C559 K560 A561 D562 D563 K564
E396 Q397 L398 G399 E400 Y401 K402 F403 Q404 L408 V409 T412 K413 P416 Q417 V418 S419 T420 L423 V424 R428 V433 C438 P447 E450 D451 Y452 V455 V456 L457 N458 Q459 V462 L463 H464 E465 V469 R472 K475 T478 E479 S480 L481 V482 N483
E292 V293 D296 E297 A300 L305 E311 S312 K313 D314 N318 Y319 K323 D324 Y332 E333 R336 S342 V343 V344 L347 R348 A364 D365 P366 H367 Y370 A371 K372 V373 F374 D375 K378 P379 L380 V381 E382 E383 P384 L387 I388 C392 E393 L394 F395

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.32Å 55.44Å 120.14Å 81.19° 90.34° 65.93°	Depositor
Resolution (Å)	22.34 – 2.70 22.46 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (22.34-2.70) 95.9 (22.46-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.281 0.233 , 0.273	Depositor DCC
R_{free} test set	1669 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 76.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.40	1/4443 (0.0%)	0.61	2/6031 (0.0%)
1	B	0.37	0/4438	0.59	1/6028 (0.0%)
All	All	0.38	1/8881 (0.0%)	0.60	3/12059 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	LYS	C-O	5.31	1.33	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	563	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	A	564	LYS	N-CA-C	-5.63	95.79	111.00
1	B	472	ARG	NE-CZ-NH1	-5.12	117.74	120.30

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	4360	0	4059	148	0
1	B	4353	0	3993	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	34	4	0
2	B	30	0	34	2	0
All	All	8773	0	8120	312	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 18.

All (312) 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:564:LYS:O	1:A:566:THR:N	1.90	1.05
1:A:424:VAL:O	1:A:428:ARG:HG3	1.72	0.89
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.07	0.88
1:B:424:VAL:O	1:B:428:ARG:HG3	1.74	0.88
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.56	0.85
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.11	0.85
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.58	0.84
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.60	0.84
1:B:218:ARG:HD3	1:B:343:VAL:HG21	1.59	0.84
1:A:95:GLU:CB	1:A:96:PRO:HD3	2.09	0.82
1:B:556:GLU:HG3	1:B:557:LYS:H	1.45	0.80
1:A:182:LEU:O	1:A:186:ARG:HG2	1.82	0.79
1:A:342:SER:HB3	1:A:447:PRO:HA	1.65	0.77
1:B:483:ASN:O	1:B:486:PRO:HD2	1.85	0.77
1:A:200:CYS:O	1:A:204:GLN:HG3	1.84	0.77
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.69	0.74
1:A:433:VAL:HG22	1:A:452:TYR:CE2	2.22	0.74
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.28	0.73
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.53	0.73
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.24	0.73
1:A:556:GLU:HG3	1:A:557:LYS:H	1.54	0.72
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.71	0.72
1:A:311:GLU:O	1:A:367:HIS:HE1	1.73	0.71
1:A:240:LYS:O	1:A:244:GLU:HG3	1.90	0.71
1:B:480:SER:OG	1:B:483:ASN:HB2	1.91	0.70
1:A:225:LYS:HE3	1:A:297:GLU:O	1.93	0.68
1:B:39:HIS:O	1:B:43:VAL:HG23	1.92	0.68
1:A:563:ASP:O	1:A:564:LYS:CB	2.41	0.68
1:B:483:ASN:C	1:B:486:PRO:HD2	2.14	0.67
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.77	0.67
1:B:392:CYS:O	1:B:396:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:O	1:A:472:ARG:NH1	2.28	0.67
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.78	0.66
1:B:36:PHE:O	1:B:40:VAL:HG23	1.94	0.66
1:A:344:VAL:CG2	1:A:450:GLU:HG2	2.26	0.65
1:B:218:ARG:HD3	1:B:343:VAL:CG2	2.26	0.65
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.62	0.65
1:A:372:LYS:O	1:A:375:ASP:HB2	1.96	0.65
1:A:367:HIS:O	1:A:371:ALA:HB2	1.97	0.65
1:B:87:MET:HE1	1:B:105:HIS:HB3	1.79	0.65
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.79	0.65
1:B:400:GLU:O	1:B:404:GLN:HG3	1.96	0.65
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.78	0.64
1:B:81:ARG:HE	1:B:88:ALA:HB3	1.62	0.64
1:A:66:LEU:O	1:A:70:PHE:HD1	1.81	0.63
1:B:81:ARG:NE	1:B:88:ALA:HB3	2.13	0.63
1:B:42:LEU:O	1:B:46:VAL:HG23	1.97	0.63
1:B:516:LEU:O	1:B:521:ARG:NH2	2.31	0.63
1:B:319:TYR:CE1	1:B:323:LYS:HB2	2.34	0.62
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.29	0.62
1:A:483:ASN:O	1:A:486:PRO:HD2	1.99	0.62
1:B:568:PHE:CD1	1:B:568:PHE:C	2.73	0.62
1:A:556:GLU:HG3	1:A:557:LYS:N	2.15	0.62
1:B:372:LYS:O	1:B:375:ASP:HB2	1.98	0.62
1:A:567:CYS:O	1:A:571:GLU:HB2	2.00	0.61
1:B:218:ARG:NH1	1:B:343:VAL:HG23	2.14	0.61
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.82	0.61
1:B:536:LYS:O	1:B:539:ALA:HB3	2.00	0.61
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.83	0.61
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.81	0.61
1:A:61:ASN:HB3	1:A:64:LYS:HD3	1.83	0.60
1:A:152:PRO:CB	1:A:257:ARG:HH11	2.14	0.60
1:A:221:GLN:HE21	1:A:339:PRO:HA	1.66	0.60
1:B:370:TYR:O	1:B:370:TYR:HD1	1.85	0.60
1:A:95:GLU:CB	1:A:96:PRO:CD	2.80	0.60
1:A:342:SER:CB	1:A:447:PRO:HA	2.32	0.60
1:A:418:VAL:HG12	1:A:423:LEU:HG	1.83	0.59
1:A:311:GLU:O	1:A:367:HIS:CE1	2.54	0.59
1:A:555:VAL:O	1:A:559:CYS:HB2	2.03	0.59
1:A:400:GLU:O	1:A:404:GLN:HG3	2.03	0.58
1:A:507:PHE:CZ	1:A:531:GLU:HB3	2.38	0.58
1:B:19:PHE:O	1:B:23:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:O	1:A:43:VAL:HG23	2.04	0.58
1:A:206:PHE:CD2	1:A:481:LEU:HD22	2.38	0.58
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.68	0.58
1:A:563:ASP:O	1:A:564:LYS:O	2.21	0.58
1:B:556:GLU:HG3	1:B:557:LYS:N	2.18	0.58
1:B:135:LEU:HD11	1:B:162:LYS:HD3	1.84	0.57
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.18	0.57
1:A:41:LYS:O	1:A:45:GLU:HG3	2.04	0.57
1:B:23:VAL:O	1:B:27:PHE:HD1	1.87	0.57
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.87	0.57
1:B:556:GLU:O	1:B:560:LYS:HG2	2.04	0.57
1:A:384:PRO:O	1:A:388:ILE:HG12	2.04	0.57
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.85	0.57
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.34	0.57
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.39	0.57
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.57
1:B:344:VAL:HG22	1:B:451:ASP:OD1	2.05	0.56
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.87	0.56
1:B:52:THR:HA	1:B:56:ASP:OD2	2.06	0.56
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.36	0.56
1:B:194:ALA:HB1	1:B:455:VAL:HG13	1.88	0.56
1:B:568:PHE:C	1:B:568:PHE:HD1	2.10	0.56
1:B:501:GLU:OE1	1:B:501:GLU:HA	2.06	0.55
1:B:29:GLN:HG2	1:B:143:ALA:O	2.05	0.55
1:A:310:VAL:HG11	1:A:374:PHE:CE1	2.41	0.55
1:A:279:CYS:HA	1:A:286:LYS:CD	2.36	0.55
1:A:516:LEU:O	1:A:521:ARG:NH2	2.39	0.55
1:B:384:PRO:O	1:B:388:ILE:HG12	2.06	0.55
1:A:511:ALA:C	1:A:513:ILE:H	2.10	0.55
1:B:279:CYS:HA	1:B:286:LYS:HD2	1.89	0.55
1:B:290:ILE:O	1:B:293:VAL:HG12	2.07	0.55
1:A:344:VAL:HG21	1:A:450:GLU:HG2	1.89	0.55
1:B:81:ARG:HE	1:B:88:ALA:CB	2.18	0.55
1:A:408:LEU:HD22	1:A:530:VAL:HG22	1.89	0.55
1:A:153:GLU:O	1:A:157:PHE:HD1	1.90	0.54
1:B:48:GLU:O	1:B:48:GLU:HG2	2.08	0.54
1:B:333:GLU:HA	1:B:336:ARG:CD	2.38	0.54
1:A:412:THR:O	1:A:416:PRO:HG3	2.08	0.54
1:A:483:ASN:C	1:A:486:PRO:HD2	2.28	0.54
1:B:205:LYS:NZ	1:B:478:THR:HG22	2.23	0.54
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:O	1:A:533:VAL:HG23	2.07	0.54
1:B:536:LYS:O	1:B:539:ALA:CB	2.55	0.54
1:A:38:ASP:O	1:A:42:LEU:HG	2.07	0.53
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.48	0.53
1:B:563:ASP:OD2	1:B:567:CYS:HB3	2.08	0.53
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.91	0.53
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.62	0.53
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.90	0.53
1:B:433:VAL:HG22	1:B:452:TYR:CE2	2.43	0.52
1:B:279:CYS:HA	1:B:286:LYS:CD	2.39	0.52
1:B:364:ALA:O	1:B:366:PRO:HD3	2.09	0.52
1:A:49:PHE:HD2	1:A:49:PHE:O	1.92	0.52
1:B:342:SER:HB3	1:B:447:PRO:HA	1.91	0.52
1:B:503:ASN:OD1	1:B:506:THR:N	2.42	0.52
1:A:42:LEU:O	1:A:46:VAL:HG23	2.10	0.52
1:B:558:CYS:SG	1:B:568:PHE:N	2.83	0.52
1:A:117:ARG:HH21	1:A:186:ARG:NE	2.08	0.52
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.44	0.52
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.75	0.52
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.65	0.52
1:A:286:LYS:O	1:A:290:ILE:HG13	2.09	0.51
1:B:16:GLU:O	1:B:20:LYS:HG2	2.10	0.51
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.93	0.51
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.40	0.51
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.11	0.51
1:B:458:ASN:O	1:B:462:VAL:HG22	2.11	0.51
1:A:5:SER:HB3	1:A:57:GLU:HG2	1.93	0.50
1:B:311:GLU:O	1:B:367:HIS:CE1	2.63	0.50
1:B:81:ARG:HG2	1:B:88:ALA:CB	2.41	0.50
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.47	0.50
1:A:408:LEU:HD12	1:A:526:GLN:HG2	1.92	0.50
1:B:168:CYS:SG	1:B:177:CYS:C	2.90	0.50
1:A:408:LEU:CD1	1:A:526:GLN:HG2	2.42	0.50
1:B:418:VAL:HG12	1:B:423:LEU:HG	1.92	0.50
1:B:342:SER:OG	1:B:344:VAL:HG23	2.12	0.50
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.93	0.50
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.37	0.50
1:A:49:PHE:C	1:A:49:PHE:CD2	2.85	0.50
1:B:14:LEU:HD13	1:B:22:LEU:HD12	1.92	0.50
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.93	0.50
1:B:543:GLN:O	1:B:546:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:MET:O	1:B:90:CYS:HB2	2.12	0.49
1:B:342:SER:CB	1:B:447:PRO:HA	2.42	0.49
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.41	0.49
1:B:541:LYS:HA	1:B:544:LEU:HD12	1.95	0.49
1:A:305:LEU:HD21	1:A:333:GLU:CB	2.42	0.49
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.35	0.49
1:B:394:LEU:O	1:B:397:GLN:HG2	2.13	0.49
1:B:517:SER:OG	1:B:520:GLU:HG2	2.12	0.49
1:B:333:GLU:O	1:B:336:ARG:HG2	2.13	0.49
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.95	0.49
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.93	0.49
1:A:49:PHE:CE2	1:A:53:CYS:SG	3.06	0.49
1:B:218:ARG:HH11	1:B:343:VAL:CG2	2.25	0.49
1:A:333:GLU:O	1:A:336:ARG:HG2	2.12	0.48
1:B:57:GLU:HB3	1:B:58:SER:H	1.46	0.48
1:B:475:LYS:O	1:B:479:GLU:HB2	2.13	0.48
1:B:127:PHE:O	1:B:131:GLU:HB3	2.12	0.48
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.48	0.48
1:A:511:ALA:C	1:A:513:ILE:N	2.67	0.48
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.28	0.48
1:B:507:PHE:CD1	1:B:507:PHE:O	2.66	0.48
1:B:283:LEU:HG	1:B:284:LEU:HD23	1.95	0.48
1:B:347:LEU:HD22	2:B:2002:IBP:H101	1.94	0.48
1:A:426:VAL:O	1:A:430:LEU:HG	2.14	0.48
1:B:5:SER:HA	1:B:62:CYS:O	2.14	0.48
1:B:387:LEU:HD22	1:B:485:ARG:NH1	2.29	0.48
1:A:168:CYS:SG	1:A:177:CYS:C	2.93	0.48
1:A:420:THR:HB	1:A:421:PRO:HD3	1.96	0.48
1:A:433:VAL:CG1	2:A:2001:IBP:H51	2.43	0.48
1:A:543:GLN:H	1:A:543:GLN:HG2	1.46	0.48
1:A:571:GLU:N	1:A:571:GLU:OE1	2.47	0.48
1:A:350:ALA:HB1	2:A:2002:IBP:H42	1.96	0.48
1:B:507:PHE:CE1	1:B:509:PHE:CZ	3.02	0.48
1:A:526:GLN:O	1:A:530:VAL:HG23	2.14	0.47
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.36	0.47
1:B:57:GLU:O	1:B:59:ALA:N	2.47	0.47
1:B:98:ARG:O	1:B:101:CYS:HB3	2.14	0.47
1:A:173:ASP:HB3	1:A:176:ALA:HB3	1.95	0.47
1:B:370:TYR:O	1:B:370:TYR:CD1	2.64	0.47
1:A:49:PHE:HD2	1:A:49:PHE:C	2.18	0.47
1:A:464:HIS:CG	1:A:473:VAL:HG11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:SER:OG	1:B:7:VAL:HG12	2.15	0.47
1:B:314:ASP:O	1:B:318:ASN:ND2	2.48	0.47
1:B:571:GLU:HA	1:B:571:GLU:OE1	2.15	0.47
1:A:387:LEU:HD22	1:A:485:ARG:NH1	2.30	0.47
1:A:552:ALA:O	1:A:556:GLU:HG2	2.15	0.47
1:A:218:ARG:HD2	1:A:343:VAL:HG21	1.96	0.47
1:A:480:SER:OG	1:A:483:ASN:HB2	2.15	0.47
1:B:218:ARG:NH1	1:B:343:VAL:CG2	2.79	0.46
1:B:25:ILE:O	1:B:29:GLN:HG3	2.15	0.46
1:B:9:HIS:NE2	1:B:13:ASP:OD2	2.48	0.46
1:A:100:GLU:HA	1:A:100:GLU:OE1	2.15	0.46
1:A:252:GLU:OE1	1:A:252:GLU:N	2.36	0.46
1:B:75:CYS:HA	1:B:78:ALA:HB3	1.97	0.46
1:A:279:CYS:HA	1:A:286:LYS:HD3	1.97	0.46
1:A:306:ALA:CA	1:A:310:VAL:HG22	2.44	0.46
1:B:323:LYS:HG3	1:B:324:ASP:N	2.29	0.46
1:A:87:MET:HE1	1:A:105:HIS:CB	2.41	0.46
1:A:507:PHE:HZ	1:A:535:HIS:CD2	2.33	0.46
1:B:51:LYS:C	1:B:53:CYS:H	2.19	0.46
1:B:285:GLU:O	1:B:289:CYS:HB2	2.16	0.46
1:A:66:LEU:HB3	1:A:70:PHE:CE1	2.51	0.46
1:A:417:GLN:H	1:A:417:GLN:CD	2.20	0.46
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.70	0.46
1:B:283:LEU:HG	1:B:284:LEU:N	2.31	0.46
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.46	0.46
1:A:507:PHE:CZ	1:A:535:HIS:CD2	3.04	0.46
1:B:73:LYS:O	1:B:76:THR:HG23	2.16	0.45
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.98	0.45
1:B:568:PHE:CD1	1:B:569:ALA:N	2.85	0.45
1:A:244:GLU:OE1	1:A:256:ASP:OD2	2.35	0.45
1:B:502:PHE:CE1	1:B:507:PHE:CE2	3.05	0.45
1:A:61:ASN:O	1:A:63:ASP:N	2.50	0.45
1:A:502:PHE:CE1	1:A:504:ALA:HA	2.52	0.45
1:B:367:HIS:O	1:B:371:ALA:HB2	2.16	0.45
1:A:117:ARG:O	1:A:117:ARG:HG3	2.17	0.45
1:A:446:MET:N	1:A:447:PRO:HD2	2.31	0.45
1:B:6:GLU:O	1:B:10:ARG:HG2	2.17	0.45
1:B:296:ASP:OD1	1:B:297:GLU:N	2.49	0.45
1:B:240:LYS:HE2	1:B:244:GLU:OE2	2.16	0.45
1:A:430:LEU:O	1:A:433:VAL:HG23	2.16	0.45
1:B:554:PHE:CD2	1:B:571:GLU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.52	0.44
1:B:456:VAL:O	1:B:459:GLN:HB2	2.18	0.44
1:A:213:ALA:HB1	1:A:347:LEU:CD2	2.47	0.44
1:B:113:PRO:O	1:B:114:ARG:O	2.35	0.44
1:B:418:VAL:CG1	1:B:423:LEU:HG	2.47	0.44
1:B:502:PHE:HE1	1:B:507:PHE:CE2	2.34	0.44
1:A:135:LEU:HD11	1:A:162:LYS:CG	2.47	0.44
1:A:23:VAL:O	1:A:27:PHE:HD1	2.00	0.44
1:A:117:ARG:HH21	1:A:186:ARG:HE	1.66	0.44
1:B:333:GLU:HA	1:B:336:ARG:HD3	1.98	0.44
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.00	0.44
1:B:187:ASP:O	1:B:190:LYS:N	2.50	0.44
1:B:510:HIS:CB	1:B:512:ASP:OD1	2.65	0.44
1:B:381:VAL:O	1:B:384:PRO:HD2	2.17	0.44
1:B:412:THR:O	1:B:416:PRO:HG3	2.18	0.44
1:A:225:LYS:HD3	1:A:299:PRO:HG3	2.00	0.44
1:A:418:VAL:CG1	1:A:423:LEU:HG	2.48	0.44
1:B:370:TYR:CD1	1:B:370:TYR:C	2.91	0.44
1:A:25:ILE:O	1:A:29:GLN:HG3	2.18	0.43
1:B:511:ALA:C	1:B:513:ILE:H	2.19	0.43
1:A:21:ALA:HB1	1:A:155:LEU:HD21	1.99	0.43
1:A:511:ALA:O	1:A:513:ILE:N	2.51	0.43
1:B:61:ASN:HB3	1:B:64:LYS:HE2	2.00	0.43
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.99	0.43
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.33	0.43
1:A:566:THR:C	1:A:568:PHE:N	2.71	0.43
1:A:464:HIS:HE1	1:A:470:SER:H	1.64	0.43
1:B:37:GLU:CD	1:B:37:GLU:H	2.21	0.43
1:B:312:SER:O	1:B:367:HIS:HE1	2.01	0.43
1:B:364:ALA:C	1:B:366:PRO:HD3	2.39	0.43
1:B:409:VAL:O	1:B:413:LYS:HG3	2.17	0.43
1:B:344:VAL:HG21	1:B:450:GLU:HG2	2.00	0.43
1:A:290:ILE:O	1:A:293:VAL:HG12	2.19	0.42
1:B:32:GLN:NE2	1:B:110:PRO:HG3	2.33	0.42
1:A:49:PHE:HE2	1:A:53:CYS:SG	2.42	0.42
1:A:66:LEU:HD13	1:A:66:LEU:N	2.34	0.42
1:A:489:SER:OG	2:A:2001:IBP:C7	2.67	0.42
1:B:21:ALA:O	1:B:25:ILE:HG13	2.19	0.42
1:B:161:TYR:CZ	1:B:165:PHE:HE2	2.36	0.42
1:B:542:GLU:O	1:B:544:LEU:N	2.53	0.42
1:A:453:LEU:HD11	2:A:2001:IBP:H53	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:HIS:CE1	1:A:469:VAL:H	2.37	0.42
1:A:531:GLU:O	1:A:535:HIS:CD2	2.72	0.42
1:B:464:HIS:CE1	1:B:469:VAL:H	2.38	0.42
1:B:179:LEU:CB	1:B:180:PRO:HD3	2.50	0.42
1:B:398:LEU:HB3	1:B:402:LYS:CB	2.50	0.42
1:A:150:TYR:O	1:A:153:GLU:HB2	2.20	0.42
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.52	0.42
1:B:46:VAL:HG22	1:B:73:LYS:HE3	2.02	0.42
1:B:141:GLU:HA	1:B:141:GLU:OE1	2.20	0.42
1:B:70:PHE:N	1:B:70:PHE:CD1	2.88	0.42
1:B:135:LEU:O	1:B:138:TYR:HB3	2.19	0.42
1:A:37:GLU:CD	1:A:37:GLU:H	2.22	0.41
1:B:81:ARG:HA	1:B:84:TYR:O	2.20	0.41
1:B:212:LYS:O	1:B:216:VAL:HG23	2.19	0.41
1:B:565:GLU:CB	1:B:568:PHE:CE2	3.03	0.41
1:B:420:THR:HG21	1:B:527:THR:HG23	2.02	0.41
1:B:576:VAL:O	1:B:579:SER:OG	2.37	0.41
1:B:34:CYS:HA	1:B:35:PRO:HD3	1.89	0.41
1:A:222:ARG:C	1:A:224:PRO:HD3	2.40	0.41
1:B:23:VAL:O	1:B:27:PHE:CD1	2.71	0.41
1:A:66:LEU:O	1:A:70:PHE:CD1	2.69	0.41
1:A:61:ASN:C	1:A:63:ASP:N	2.74	0.41
1:A:61:ASN:C	1:A:63:ASP:H	2.24	0.41
1:A:99:ASN:O	1:A:103:LEU:HG	2.21	0.41
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.92	0.41
1:B:218:ARG:HD2	1:B:218:ARG:HA	1.79	0.41
1:B:314:ASP:HB3	1:B:318:ASN:HD21	1.86	0.41
1:B:518:GLU:O	1:B:521:ARG:HB3	2.21	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.87	0.41
1:A:298:MET:HA	1:A:299:PRO:HD3	1.94	0.40
1:B:332:TYR:O	1:B:336:ARG:HD2	2.21	0.40
1:B:81:ARG:HG2	1:B:88:ALA:HB3	2.02	0.40
1:B:482:VAL:HG23	2:B:2002:IBP:O1	2.21	0.40
1:B:237:ASP:HB2	1:B:260:LEU:HD13	2.03	0.40
1:B:482:VAL:O	1:B:482:VAL:HG12	2.20	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%)	507 (88%)	54 (9%)	15 (3%)	5 13
1	B	576/585 (98%)	508 (88%)	51 (9%)	17 (3%)	4 10
All	All	1152/1170 (98%)	1015 (88%)	105 (9%)	32 (3%)	5 11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	95	GLU
1	A	300	ALA
1	A	565	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	114	ARG
1	B	566	THR
1	A	58	SER
1	A	502	PHE
1	B	85	GLY
1	B	300	ALA
1	B	543	GLN
1	A	17	GLU
1	A	62	CYS
1	A	312	SER
1	A	539	ALA
1	B	60	GLU
1	B	565	GLU
1	A	564	LYS
1	B	167	GLU
1	B	188	GLU
1	B	438	CYS
1	B	465	GLU

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Mol	Chain	Res	Type
1	B	542	GLU
1	A	57	GLU
1	A	179	LEU
1	B	77	VAL
1	B	150	TYR
1	A	315	VAL
1	A	118	PRO

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	444/511 (87%)	428 (96%)	16 (4%)	35	64
1	B	437/511 (86%)	422 (97%)	15 (3%)	37	66
All	All	881/1022 (86%)	850 (96%)	31 (4%)	36	65

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	30	TYR
1	A	37	GLU
1	A	49	PHE
1	A	66	LEU
1	A	72	ASP
1	A	79	THR
1	A	109	ASN
1	A	111	ASN
1	A	245	CYS
1	A	336	ARG
1	A	375	ASP
1	A	471	ASP
1	A	480	SER
1	A	543	GLN
1	A	550	ASP

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Mol	Chain	Res	Type
1	B	38	ASP
1	B	56	ASP
1	B	57	GLU
1	B	79	THR
1	B	82	GLU
1	B	245	CYS
1	B	292	GLU
1	B	323	LYS
1	B	344	VAL
1	B	375	ASP
1	B	480	SER
1	B	489	SER
1	B	532	LEU
1	B	550	ASP
1	B	568	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	99	ASN
1	A	109	ASN
1	A	111	ASN
1	A	196	GLN
1	A	221	GLN
1	A	318	ASN
1	A	367	HIS
1	A	429	ASN
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	B	196	GLN
1	B	318	ASN
1	B	338	HIS
1	B	385	GLN
1	B	464	HIS
1	B	483	ASN

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)

4 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	IBP	A	2002	-	15,15,15	2.66	8 (53%)	20,20,20	1.29	1 (5%)
2	IBP	B	2001	-	15,15,15	1.84	5 (33%)	20,20,20	0.86	1 (5%)
2	IBP	B	2002	-	15,15,15	2.39	7 (46%)	20,20,20	1.15	1 (5%)
2	IBP	A	2001	-	15,15,15	1.70	4 (26%)	20,20,20	0.84	1 (5%)

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	IBP	A	2002	-	-	7/12/12/12	0/1/1/1
2	IBP	B	2001	-	-	5/12/12/12	0/1/1/1
2	IBP	B	2002	-	-	5/12/12/12	0/1/1/1
2	IBP	A	2001	-	-	4/12/12/12	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	IBP	C13-C8	4.42	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	IBP	C8-C6	4.28	1.59	1.52
2	B	2002	IBP	C13-C8	4.18	1.45	1.39
2	A	2002	IBP	C13-C12	4.14	1.46	1.38
2	B	2002	IBP	C13-C12	3.81	1.45	1.38
2	A	2002	IBP	C9-C8	3.54	1.44	1.39
2	A	2002	IBP	C10-C9	3.41	1.45	1.38
2	B	2002	IBP	C8-C6	3.41	1.58	1.52
2	A	2001	IBP	C10-C11	3.40	1.46	1.38
2	B	2002	IBP	C9-C8	3.39	1.44	1.39
2	B	2002	IBP	C10-C9	3.29	1.44	1.38
2	A	2001	IBP	C13-C8	3.20	1.44	1.39
2	A	2002	IBP	C12-C11	3.18	1.45	1.38
2	B	2001	IBP	C9-C8	3.10	1.44	1.39
2	A	2002	IBP	C10-C11	3.10	1.45	1.38
2	B	2001	IBP	C13-C8	3.01	1.43	1.39
2	B	2001	IBP	C10-C11	2.92	1.45	1.38
2	B	2001	IBP	C10-C9	2.88	1.44	1.38
2	B	2002	IBP	C10-C11	2.76	1.44	1.38
2	B	2002	IBP	C12-C11	2.73	1.44	1.38
2	A	2001	IBP	C9-C8	2.63	1.43	1.39
2	B	2001	IBP	C13-C12	2.40	1.43	1.38
2	A	2001	IBP	C10-C9	2.32	1.43	1.38
2	A	2002	IBP	C2-C11	2.32	1.56	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	IBP	C7-C6-C8	4.33	123.30	112.92
2	B	2002	IBP	C7-C6-C8	4.03	122.58	112.92
2	B	2001	IBP	C7-C6-C8	3.10	120.35	112.92
2	A	2001	IBP	C7-C6-C8	2.87	119.80	112.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2002	IBP	C10-C11-C2-C3
2	A	2002	IBP	C12-C11-C2-C3
2	A	2001	IBP	O2-C1-C6-C8
2	B	2001	IBP	C11-C2-C3-C5
2	A	2001	IBP	O1-C1-C6-C8
2	A	2002	IBP	O1-C1-C6-C8

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Mol	Chain	Res	Type	Atoms
2	A	2002	IBP	O2-C1-C6-C8
2	A	2001	IBP	C10-C11-C2-C3
2	B	2001	IBP	O1-C1-C6-C8
2	B	2002	IBP	C11-C2-C3-C5
2	A	2001	IBP	C12-C11-C2-C3
2	B	2002	IBP	O1-C1-C6-C7
2	B	2002	IBP	O2-C1-C6-C7
2	A	2002	IBP	O1-C1-C6-C7
2	B	2001	IBP	O2-C1-C6-C7
2	B	2001	IBP	O2-C1-C6-C8
2	B	2002	IBP	O2-C1-C6-C8
2	A	2002	IBP	O2-C1-C6-C7
2	B	2001	IBP	O1-C1-C6-C7
2	B	2002	IBP	O1-C1-C6-C8
2	A	2002	IBP	C11-C2-C3-C5

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	IBP	1	0
2	B	2002	IBP	2	0
2	A	2001	IBP	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	578/585 (98%)	0.15	37 (6%)	19	18	29, 70, 136, 146	0
1	B	578/585 (98%)	0.17	42 (7%)	15	13	25, 72, 137, 151	0
All	All	1156/1170 (98%)	0.16	79 (6%)	17	15	25, 71, 137, 151	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	562	ASP	8.1
1	B	566	THR	7.8
1	B	555	VAL	6.7
1	A	572	GLY	6.4
1	A	569	ALA	5.9
1	A	554	PHE	5.6
1	A	555	VAL	5.5
1	B	82	GLU	5.4
1	A	83	THR	5.3
1	A	570	GLU	5.0
1	B	83	THR	4.9
1	A	581	ALA	4.7
1	A	79	THR	4.6
1	B	509	PHE	4.6
1	B	512	ASP	4.4
1	A	562	ASP	4.4
1	B	572	GLY	4.3
1	A	578	ALA	4.2
1	A	551	PHE	4.2
1	B	171	ALA	4.2
1	B	506	THR	4.2
1	A	82	GLU	4.2
1	B	172	ALA	4.1
1	B	505	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	511	ALA	4.0
1	A	509	PHE	4.0
1	A	561	ALA	3.9
1	B	560	LYS	3.9
1	B	569	ALA	3.9
1	B	508	THR	3.9
1	B	510	HIS	3.8
1	A	560	LYS	3.8
1	B	515	THR	3.6
1	B	56	ASP	3.6
1	A	81	ARG	3.5
1	B	559	CYS	3.5
1	A	559	CYS	3.5
1	A	300	ALA	3.4
1	A	510	HIS	3.4
1	B	513	ILE	3.4
1	B	561	ALA	3.4
1	A	558	CYS	3.4
1	A	579	SER	3.3
1	B	300	ALA	3.2
1	A	568	PHE	3.1
1	A	85	GLY	3.0
1	B	507	PHE	3.0
1	A	87	MET	3.0
1	A	516	LEU	3.0
1	A	563	ASP	2.9
1	A	364	ALA	2.8
1	B	516	LEU	2.8
1	A	508	THR	2.8
1	A	506	THR	2.8
1	B	548	MET	2.7
1	A	564	LYS	2.6
1	B	70	PHE	2.6
1	B	84	TYR	2.6
1	B	576	VAL	2.6
1	A	84	TYR	2.5
1	A	78	ALA	2.5
1	B	55	ALA	2.4
1	B	577	ALA	2.4
1	B	558	CYS	2.4
1	B	504	ALA	2.4
1	B	573	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	2.4
1	A	511	ALA	2.4
1	B	28	ALA	2.3
1	B	121	ASP	2.3
1	B	568	PHE	2.3
1	A	26	ALA	2.3
1	B	97	GLU	2.3
1	B	554	PHE	2.2
1	B	563	ASP	2.2
1	B	79	THR	2.2
1	A	27	PHE	2.2
1	B	120	VAL	2.1
1	A	457	LEU	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	IBP	A	2002	15/15	0.83	0.29	88,90,93,94	0
2	IBP	A	2001	15/15	0.88	0.34	69,72,78,79	0
2	IBP	B	2002	15/15	0.89	0.25	99,102,103,104	0
2	IBP	B	2001	15/15	0.92	0.30	66,69,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.