WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID	:	1G50
Title	:	CRYSTAL STRUCTURE OF A WILD TYPE HER ALPHA LBD AT 2.9 ANGSTROM RESOLUTION
Authors	:	Eiler, S.; Gangloff, M.; Duclaud, S.; Moras, D.; Ruff, M.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2000-10-30
Resolution	:	2.90 Å(reported)

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 (i)

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

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.308
Clashscore		44
Ramachandran outliers		4.7%
Sidechain outliers		9.9%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
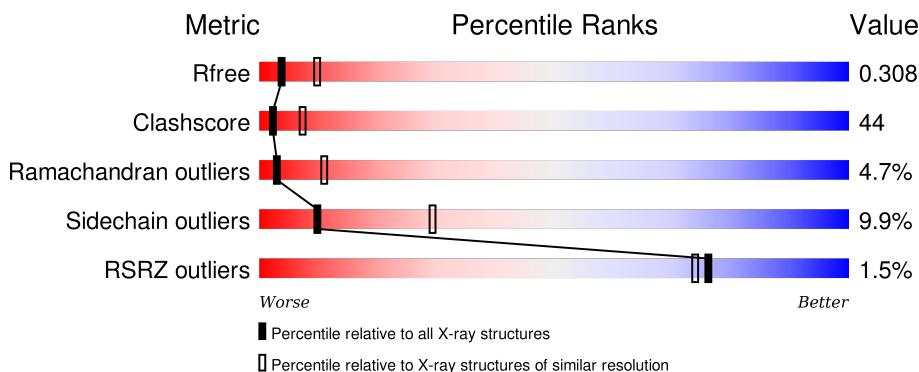
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	247	29% 59% 11% •
1	B	247	% 36% 57% • •
1	C	247	3% 37% 54% 6% • •
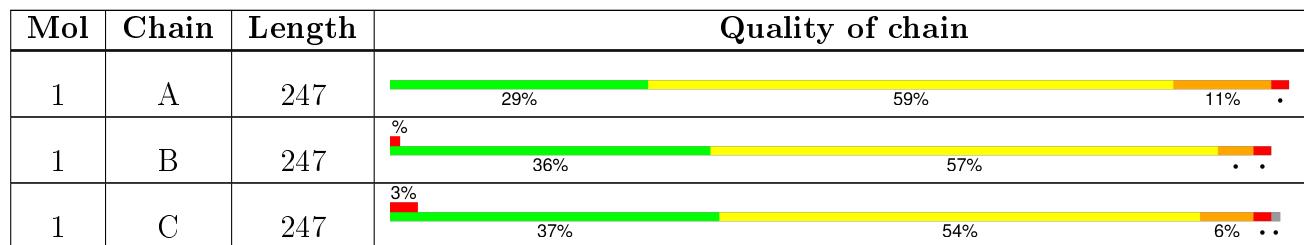
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6109 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 ESTROGEN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1975	1264	338	354	19			
1	B	246	Total	C	N	O	S	0	0	0
			1964	1258	335	352	19			
1	C	244	Total	C	N	O	S	0	0	0
			1945	1246	330	350	19			

- Molecule 2 is ESTRADIOL (three-letter code: EST) (formula: $C_{18}H_{24}O_2$).
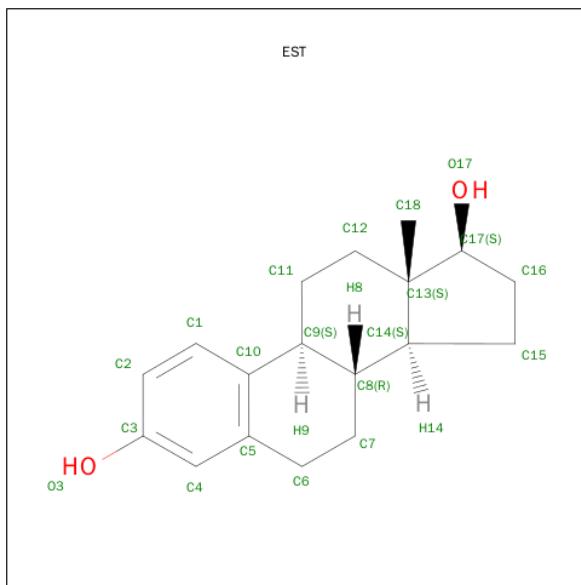
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	2		
2	C	1	Total	C	O	0	0
			20	18	2		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	53	Total 53	O 53	0	0
3	C	55	Total 55	O 55	0	0

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: ESTROGEN RECEPTOR
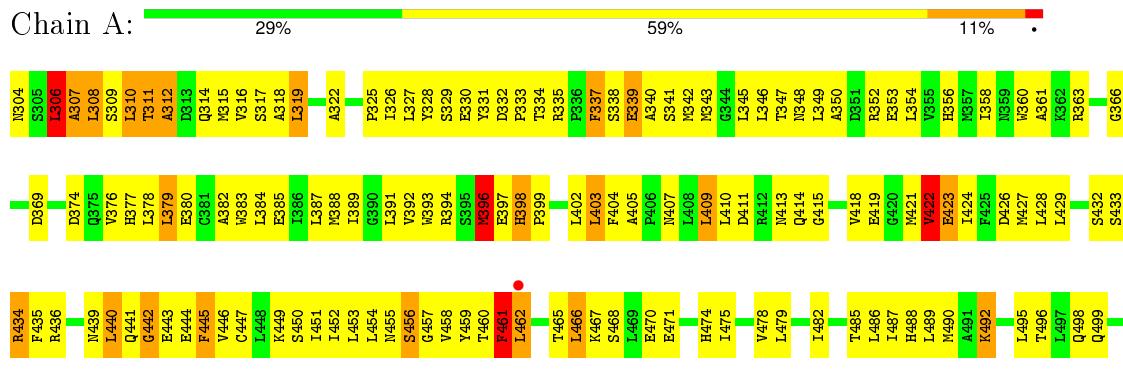
- Molecule 1: ESTROGEN RECEPTOR

- Molecule 1: ESTROGEN RECEPTOR
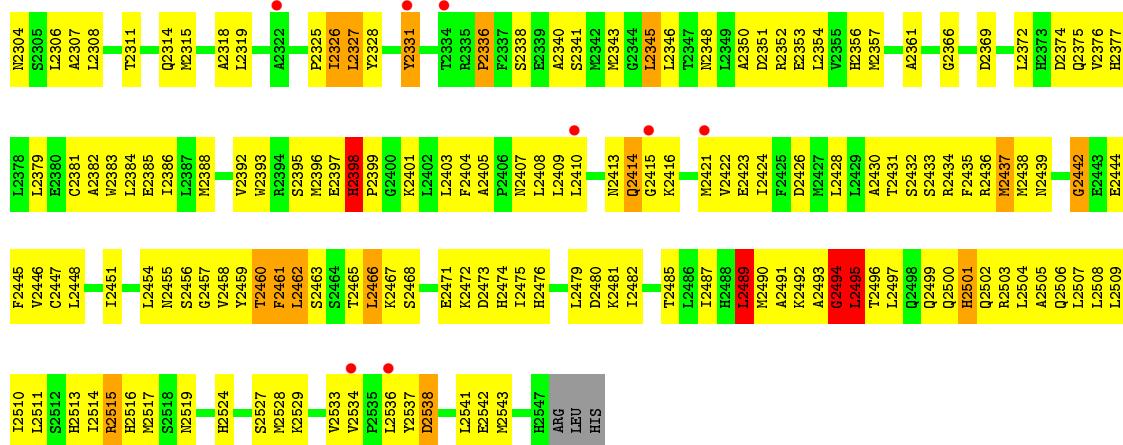
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.50Å 105.50Å 136.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.18 – 2.90 49.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.18-2.90) 91.0 (49.18-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	8.00	Depositor
$< I/\sigma(I) >$ [1]	2.61 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.310 0.243 , 0.308	Depositor DCC
R_{free} test set	1778 reflections (9.80%)	DCC
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 18142 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6109	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.52	2/2013 (0.1%)	0.74	2/2720 (0.1%)
1	B	0.76	2/2001 (0.1%)	0.72	5/2705 (0.2%)
1	C	0.68	1/1982 (0.1%)	0.69	3/2680 (0.1%)
All	All	0.66	5/5996 (0.1%)	0.72	10/8105 (0.1%)

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	2
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2495	LEU	N-CA	26.00	1.98	1.46
1	B	1310	LEU	N-CA	23.00	1.92	1.46
1	B	1327	LEU	N-CA	18.79	1.83	1.46
1	A	548	ARG	N-CA	6.64	1.59	1.46
1	A	461	PHE	N-CA	5.12	1.56	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2494	GLY	C-N-CA	-11.12	93.89	121.70
1	A	548	ARG	N-CA-CB	11.12	130.62	110.60
1	B	1309	SER	C-N-CA	-10.34	95.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2495	LEU	N-CA-CB	-9.75	90.90	110.40
1	B	1310	LEU	N-CA-C	-8.91	86.94	111.00
1	B	1326	ILE	C-N-CA	-8.50	100.46	121.70
1	B	1327	LEU	N-CA-C	-7.77	90.02	111.00
1	C	2495	LEU	N-CA-C	-6.89	92.39	111.00
1	B	1327	LEU	N-CA-CB	-5.22	99.96	110.40
1	A	461	PHE	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1309	SER	Peptide
1	B	1326	ILE	Peptide
1	C	2494	GLY	Peptide

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	1975	0	2025	206	0
1	B	1964	0	2018	175	0
1	C	1945	0	1994	170	0
2	A	20	0	24	2	0
2	B	20	0	24	2	0
2	C	20	0	24	1	0
3	A	57	0	0	10	0
3	B	53	0	0	2	0
3	C	55	0	0	5	0
All	All	6109	0	6109	525	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 44.

All (525) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:LEU:CA	1:B:1327:LEU:N	1.83	1.38
1:B:1310:LEU:N	1:B:1310:LEU:CA	1.92	1.32
1:B:1327:LEU:N	1:B:1327:LEU:HD23	1.46	1.27
1:C:2495:LEU:CA	1:C:2495:LEU:N	1.98	1.27
1:B:1327:LEU:H	1:B:1327:LEU:CD2	1.62	1.12
1:B:1328:TYR:HB3	1:B:1407:ASN:HD21	1.17	1.07
1:A:515:ARG:HG2	1:A:515:ARG:HH11	1.20	1.02
1:B:1308:LEU:HD21	1:B:1477:ARG:HD3	1.41	0.99
1:C:2311:THR:HG23	1:C:2314:GLN:HE21	1.27	0.99
1:B:1328:TYR:HB3	1:B:1407:ASN:ND2	1.78	0.98
1:B:1311:THR:HG23	1:B:1314:GLN:HE21	1.28	0.98
1:B:1504:LEU:HD23	1:C:2504:LEU:HD23	1.45	0.97
1:B:1519:ASN:HD22	1:C:2519:ASN:HD22	0.99	0.94
1:B:1519:ASN:ND2	1:C:2519:ASN:HD22	1.66	0.92
1:A:392:VAL:HG13	1:A:432:SER:HA	1.49	0.92
1:B:1327:LEU:CD2	1:B:1327:LEU:N	2.28	0.91
1:C:2457:GLY:HA2	1:C:2460:THR:HG23	1.50	0.90
1:B:1519:ASN:HD22	1:C:2519:ASN:ND2	1.69	0.89
1:A:366:GLY:HA2	1:A:369:ASP:OD2	1.74	0.88
1:C:2466:LEU:H	1:C:2466:LEU:HD13	1.36	0.88
1:A:339:GLU:O	1:A:339:GLU:HG2	1.74	0.87
1:C:2311:THR:OG1	1:C:2314:GLN:HG3	1.76	0.86
1:A:343:MET:O	1:A:347:THR:HG23	1.75	0.86
1:B:1309:SER:C	1:B:1310:LEU:CA	2.44	0.85
1:C:2494:GLY:C	1:C:2495:LEU:CA	2.46	0.84
1:B:1326:ILE:C	1:B:1327:LEU:CA	2.45	0.83
1:C:2466:LEU:HD22	1:C:2467:LYS:H	1.41	0.83
1:C:2466:LEU:HD22	1:C:2467:LYS:N	1.94	0.83
1:B:1310:LEU:H	1:B:1481:LYS:HE3	1.44	0.82
1:B:1311:THR:OG1	1:B:1314:GLN:HG3	1.79	0.82
1:A:487:ILE:HA	1:A:490:MET:HE3	1.61	0.82
1:B:1326:ILE:HG12	1:B:1326:ILE:O	1.81	0.81
1:B:1385:GLU:OE1	1:B:1515:ARG:HG2	1.79	0.81
1:C:2357:MET:HE1	1:C:2386:ILE:HB	1.63	0.80
1:B:1515:ARG:HH11	1:B:1515:ARG:HG3	1.47	0.80
1:A:329:SER:H	1:A:407:ASN:ND2	1.80	0.79
1:C:2311:THR:HG23	1:C:2314:GLN:NE2	1.98	0.77
1:A:329:SER:N	1:A:407:ASN:HD21	1.82	0.77
1:B:1311:THR:HG23	1:B:1314:GLN:NE2	1.99	0.77
1:B:1310:LEU:N	1:B:1310:LEU:C	2.38	0.77
1:C:2515:ARG:HG3	1:C:2515:ARG:HH11	1.49	0.77
1:C:2328:TYR:HB3	1:C:2407:ASN:HD21	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD23	1:A:352:ARG:NH1	1.99	0.76
1:C:2351:ASP:OD2	1:C:2537:TYR:HB3	1.86	0.75
1:B:1327:LEU:C	1:B:1327:LEU:N	2.39	0.74
1:C:2327:LEU:HA	3:C:3087:HOH:O	1.88	0.74
1:C:2385:GLU:OE1	1:C:2515:ARG:HG2	1.88	0.73
1:B:1311:THR:CG2	1:B:1314:GLN:HE21	2.01	0.73
1:A:338:SER:H	1:A:341:SER:HB3	1.52	0.73
1:A:403:LEU:HA	1:A:409:LEU:HD22	1.69	0.73
1:C:2311:THR:CG2	1:C:2314:GLN:HE21	2.00	0.72
1:C:2495:LEU:N	1:C:2495:LEU:CB	2.53	0.71
1:B:1308:LEU:HD21	1:B:1477:ARG:CD	2.20	0.71
1:B:1327:LEU:H	1:B:1327:LEU:HD23	0.68	0.71
1:B:1338:SER:H	1:B:1341:SER:HB3	1.54	0.71
1:B:1331:TYR:HB2	1:B:1345:LEU:HD11	1.73	0.70
1:B:1351:ASP:OD2	1:B:1537:TYR:HB3	1.91	0.70
1:B:1392:VAL:HG13	1:B:1432:SER:HA	1.73	0.70
1:C:2466:LEU:CD1	1:C:2466:LEU:H	2.05	0.69
1:A:515:ARG:CG	1:A:515:ARG:HH11	2.01	0.69
1:A:338:SER:C	1:A:340:ALA:H	1.96	0.69
1:C:2401:LYS:HD3	1:C:2409:LEU:HD11	1.74	0.69
1:A:382:ALA:HB2	1:A:456:SER:HB2	1.73	0.69
1:B:1326:ILE:H	1:B:1326:ILE:HD13	1.56	0.68
1:C:2392:VAL:HG13	1:C:2432:SER:HA	1.74	0.68
1:A:498:GLN:O	1:A:502:GLN:HG3	1.93	0.68
1:B:1401:LYS:HB3	1:B:1409:LEU:HD11	1.76	0.68
1:B:1310:LEU:N	1:B:1310:LEU:O	2.27	0.68
1:C:2401:LYS:HB3	1:C:2409:LEU:HD11	1.76	0.67
1:A:515:ARG:HG2	1:A:515:ARG:NH1	1.97	0.67
1:C:2466:LEU:HD13	1:C:2466:LEU:N	2.10	0.67
1:A:535:PRO:HB2	1:A:537:TYR:CE1	2.29	0.67
1:A:329:SER:H	1:A:407:ASN:HD21	1.35	0.67
1:B:1308:LEU:HD11	1:B:1477:ARG:HD2	1.77	0.66
1:A:329:SER:C	1:A:331:TYR:H	1.97	0.66
1:B:1388:MET:HG2	2:B:1600:EST:H62	1.78	0.66
1:A:378:LEU:HD23	1:A:453:LEU:O	1.96	0.66
1:B:1372:LEU:O	1:B:1376:VAL:HG23	1.96	0.66
1:C:2457:GLY:HA2	1:C:2460:THR:CG2	2.26	0.65
1:B:1381:CYS:SG	3:C:3030:HOH:O	2.54	0.65
1:B:1357:MET:HE1	1:B:1386:ILE:HB	1.79	0.65
1:C:2346:LEU:HD22	1:C:2404:PHE:CD2	2.31	0.65
1:B:1346:LEU:HD22	1:B:1404:PHE:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1401:LYS:HD3	1:B:1409:LEU:HD11	1.77	0.64
1:A:376:VAL:O	1:A:380:GLU:HG2	1.98	0.64
1:A:427:MET:HE3	1:A:517:MET:HA	1.78	0.64
1:B:1327:LEU:CB	1:B:1327:LEU:N	2.58	0.64
1:A:348:ASN:ND2	1:A:537:TYR:OH	2.27	0.64
1:B:1487:ILE:HG21	1:C:2501:HIS:CE1	2.33	0.64
1:A:468:SER:HA	3:A:3019:HOH:O	1.98	0.64
1:A:328:TYR:CA	1:A:407:ASN:HD21	2.11	0.64
1:A:312:ALA:O	1:A:315:MET:HB3	1.98	0.63
1:A:327:LEU:HD23	1:A:352:ARG:HH11	1.62	0.63
1:C:2315:MET:HE2	1:C:2481:LYS:HG2	1.80	0.63
1:A:354:LEU:O	1:A:358:ILE:HG13	1.99	0.63
1:C:2372:LEU:O	1:C:2376:VAL:HG23	1.99	0.63
1:C:2497:LEU:HD23	1:C:2500:GLN:HE22	1.61	0.62
1:C:2448:LEU:HD22	1:C:2511:LEU:HD21	1.81	0.62
1:B:1326:ILE:H	1:B:1326:ILE:CD1	2.12	0.62
1:C:2495:LEU:N	1:C:2495:LEU:HB2	2.14	0.62
1:A:456:SER:HA	1:A:515:ARG:HH22	1.65	0.61
1:C:2489:LEU:O	1:C:2489:LEU:HD23	2.00	0.61
1:C:2529:LYS:HA	1:C:2534:VAL:CG1	2.31	0.61
1:A:427:MET:CE	1:A:517:MET:HG2	2.31	0.61
1:C:2315:MET:HG2	1:C:2485:THR:OG1	2.01	0.61
1:B:1529:LYS:HA	1:B:1534:VAL:CG1	2.31	0.60
1:A:526:TYR:CD2	1:A:549:LEU:HD21	2.36	0.60
1:A:322:ALA:O	1:A:363:ARG:NH1	2.35	0.60
1:A:419:GLU:C	1:A:421:MET:H	2.03	0.60
1:C:2397:GLU:O	1:C:2399:PRO:HD3	2.01	0.60
1:B:1397:GLU:O	1:B:1399:PRO:HD3	2.02	0.60
1:C:2361:ALA:HB2	1:C:2379:LEU:HD21	1.83	0.60
1:C:2502:GLN:O	1:C:2506:GLN:HG3	2.01	0.60
1:B:1508:LEU:CD1	1:C:2505:ALA:HA	2.32	0.60
1:B:1513:HIS:HE2	1:C:2460:THR:HG22	1.67	0.60
1:A:339:GLU:HA	1:A:418:VAL:HG22	1.84	0.60
1:B:1448:LEU:HD22	1:B:1511:LEU:HD21	1.83	0.60
1:B:1348:ASN:HA	1:B:1537:TYR:CE1	2.37	0.59
1:C:2331:TYR:HA	1:C:2345:LEU:HD21	1.83	0.59
1:B:1497:LEU:HD23	1:B:1500:GLN:HE22	1.66	0.59
1:B:1307:ALA:O	1:B:1309:SER:N	2.36	0.59
1:B:1489:LEU:O	1:B:1489:LEU:HD23	2.02	0.59
1:C:2495:LEU:C	1:C:2495:LEU:N	2.55	0.59
1:B:1513:HIS:CD2	1:C:2459:TYR:HD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1437:MET:O	1:B:1437:MET:HG2	2.03	0.58
1:B:1455:ASN:O	1:B:1458:VAL:HG12	2.03	0.58
1:C:2465:THR:HB	1:C:2466:LEU:HD13	1.85	0.58
1:A:454:LEU:HD22	1:A:475:ILE:HG23	1.84	0.58
1:C:2306:LEU:HD12	1:C:2307:ALA:N	2.18	0.58
1:B:1502:GLN:O	1:B:1506:GLN:HG3	2.04	0.58
1:B:1326:ILE:CG1	1:B:1326:ILE:O	2.52	0.57
1:A:327:LEU:HD12	1:A:327:LEU:N	2.19	0.57
1:C:2494:GLY:O	1:C:2495:LEU:CA	2.53	0.57
1:A:549:LEU:HD23	1:A:549:LEU:O	2.03	0.57
1:C:2437:MET:O	1:C:2437:MET:HG2	2.03	0.57
1:C:2538:ASP:OD2	1:C:2538:ASP:N	2.36	0.57
1:A:304:ASN:HA	1:A:308:LEU:HD12	1.85	0.57
1:A:385:GLU:HG2	1:A:518:SER:HB2	1.85	0.57
1:C:2496:THR:OG1	1:C:2499:GLN:HG3	2.04	0.57
1:B:1306:LEU:O	1:B:1306:LEU:HD23	2.04	0.57
1:B:1326:ILE:N	1:B:1326:ILE:HD13	2.19	0.57
1:B:1309:SER:O	1:B:1310:LEU:CA	2.52	0.57
1:B:1315:MET:HE2	1:B:1481:LYS:HG2	1.86	0.57
1:A:354:LEU:HD11	1:A:387:LEU:HD11	1.86	0.57
1:B:1480:ASP:OD1	1:C:2502:GLN:HB3	2.05	0.57
1:A:511:LEU:HD23	1:A:511:LEU:N	2.20	0.57
1:A:429:LEU:O	1:A:432:SER:HB3	2.05	0.57
1:C:2348:ASN:HA	1:C:2537:TYR:CE1	2.40	0.57
1:C:2396:MET:O	1:C:2436:ARG:HD3	2.04	0.57
1:B:1403:LEU:HG	1:B:1409:LEU:HD23	1.87	0.57
1:A:389:ILE:HG12	1:A:445:PHE:HE1	1.69	0.57
1:A:398:HIS:N	1:A:398:HIS:ND1	2.52	0.57
1:A:542:GLU:HG2	1:A:543:MET:HE3	1.87	0.57
1:B:1392:VAL:HG11	1:B:1431:THR:HG22	1.85	0.56
1:B:1315:MET:HG2	1:B:1485:THR:OG1	2.05	0.56
1:B:1483:THR:HG21	1:C:2502:GLN:HA	1.87	0.56
1:A:529:LYS:C	1:A:531:LYS:H	2.08	0.56
1:B:1396:MET:O	1:B:1436:ARG:HD3	2.05	0.56
1:B:1361:ALA:HB2	1:B:1379:LEU:HD21	1.87	0.56
1:B:1501:HIS:CE1	1:C:2487:ILE:HG21	2.41	0.56
1:C:2490:MET:SD	1:C:2503:ARG:HD3	2.45	0.56
1:B:1447:CYS:O	1:B:1451:ILE:HG13	2.05	0.56
1:C:2447:CYS:O	1:C:2451:ILE:HG13	2.05	0.56
1:A:455:ASN:O	1:A:456:SER:C	2.41	0.56
1:B:1490:MET:SD	1:B:1503:ARG:HD3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1310:LEU:N	1:B:1310:LEU:CB	2.68	0.56
1:A:349:LEU:HG	1:A:353:GLU:OE2	2.06	0.55
1:A:396:MET:O	1:A:436:ARG:HD3	2.07	0.55
1:C:2343:MET:HA	1:C:2343:MET:CE	2.37	0.55
1:A:383:TRP:CG	1:A:384:LEU:N	2.75	0.54
1:B:1459:TYR:HE2	1:C:2434:ARG:HH11	1.54	0.54
1:C:2327:LEU:HD12	1:C:2352:ARG:HH11	1.71	0.54
1:B:1338:SER:OG	1:B:1341:SER:HB2	2.08	0.54
1:B:1393:TRP:CZ2	1:B:1442:GLY:HA2	2.42	0.54
1:B:1327:LEU:O	1:B:1327:LEU:N	2.40	0.54
1:C:2510:ILE:O	1:C:2514:ILE:HG13	2.08	0.54
1:C:2442:GLY:O	1:C:2445:PHE:HB3	2.08	0.54
1:A:329:SER:O	1:A:331:TYR:N	2.38	0.54
1:B:1523:GLU:OE2	1:B:1549:LEU:HG	2.07	0.54
1:C:2403:LEU:HG	1:C:2409:LEU:HD23	1.89	0.54
1:C:2392:VAL:HG11	1:C:2431:THR:HG22	1.88	0.54
1:A:458:VAL:HG13	1:A:459:TYR:N	2.23	0.54
1:B:1329:SER:HA	1:B:1352:ARG:HH22	1.73	0.54
1:A:487:ILE:HD13	1:A:490:MET:CE	2.38	0.54
1:B:1515:ARG:HG3	1:B:1515:ARG:NH1	2.20	0.54
1:A:385:GLU:HG2	1:A:518:SER:CB	2.37	0.54
1:A:495:LEU:HB3	1:A:499:GLN:HB2	1.90	0.54
1:C:2515:ARG:HG3	1:C:2515:ARG:NH1	2.22	0.54
1:C:2455:ASN:O	1:C:2458:VAL:HG12	2.08	0.54
1:A:396:MET:HE2	1:A:440:LEU:HB3	1.90	0.54
1:B:1343:MET:CE	1:B:1343:MET:HA	2.37	0.54
1:B:1409:LEU:HD13	1:B:1410:LEU:N	2.23	0.53
1:A:358:ILE:O	1:A:361:ALA:HB3	2.08	0.53
1:C:2393:TRP:CZ2	1:C:2442:GLY:HA2	2.42	0.53
1:A:337:PHE:CD1	1:A:337:PHE:N	2.76	0.53
1:B:1448:LEU:HD11	1:B:1507:LEU:HD22	1.90	0.53
1:C:2506:GLN:O	1:C:2510:ILE:HG12	2.09	0.53
1:A:326:ILE:N	1:A:326:ILE:HD12	2.24	0.53
1:A:426:ASP:HA	1:A:429:LEU:HD12	1.90	0.53
1:B:1442:GLY:O	1:B:1445:PHE:HB3	2.08	0.53
1:B:1325:PRO:HG2	1:B:1356:HIS:ND1	2.24	0.53
1:A:338:SER:O	1:A:340:ALA:N	2.41	0.53
1:B:1538:ASP:OD2	1:B:1538:ASP:N	2.37	0.53
1:C:2340:ALA:HA	1:C:2533:VAL:CG1	2.39	0.53
1:A:465:THR:O	1:A:468:SER:HB3	2.08	0.53
1:C:2338:SER:H	1:C:2341:SER:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:THR:HG23	1:A:499:GLN:OE1	2.08	0.52
1:A:535:PRO:HB2	1:A:537:TYR:CD1	2.45	0.52
1:B:1506:GLN:O	1:B:1510:ILE:HG12	2.08	0.52
1:C:2491:ALA:C	1:C:2493:ALA:H	2.12	0.52
1:A:496:THR:HG23	1:A:499:GLN:CD	2.30	0.52
1:A:536:LEU:HD12	1:A:536:LEU:H	1.75	0.52
1:A:329:SER:HB3	1:A:407:ASN:OD1	2.09	0.52
1:B:1476:HIS:NE2	1:C:2434:ARG:NH1	2.57	0.52
1:A:402:LEU:O	1:A:404:PHE:N	2.42	0.52
1:B:1459:TYR:HB3	1:C:2430:ALA:HB1	1.92	0.52
1:B:1340:ALA:HA	1:B:1533:VAL:CG1	2.39	0.52
1:A:311:THR:HG23	1:A:314:GLN:OE1	2.09	0.52
1:A:327:LEU:HB3	1:A:352:ARG:HH12	1.74	0.52
1:A:388:MET:HG2	1:A:428:LEU:HD21	1.91	0.52
1:A:306:LEU:O	1:A:307:ALA:C	2.47	0.52
1:A:397:GLU:HB3	1:A:398:HIS:ND1	2.25	0.52
1:C:2448:LEU:HD11	1:C:2507:LEU:CD2	2.40	0.51
1:C:2529:LYS:HA	1:C:2534:VAL:HG12	1.91	0.51
1:C:2415:GLY:O	1:C:2421:MET:HB3	2.10	0.51
1:B:1415:GLY:O	1:B:1421:MET:HB3	2.09	0.51
1:B:1524:HIS:O	1:B:1527:SER:HB3	2.10	0.51
1:C:2405:ALA:HB3	1:C:2408:LEU:HB3	1.92	0.51
1:A:342:MET:O	1:A:343:MET:C	2.48	0.51
1:C:2325:PRO:HG2	1:C:2356:HIS:ND1	2.26	0.51
1:A:338:SER:C	1:A:340:ALA:N	2.63	0.51
1:A:393:TRP:O	1:A:396:MET:HB2	2.11	0.51
1:A:515:ARG:NH1	1:A:515:ARG:CG	2.64	0.51
1:A:382:ALA:HB1	1:A:452:ILE:HG22	1.93	0.51
1:B:1392:VAL:HG13	1:B:1432:SER:CA	2.40	0.51
1:C:2448:LEU:HD11	1:C:2507:LEU:HD22	1.93	0.51
1:B:1529:LYS:HA	1:B:1534:VAL:HG12	1.91	0.51
1:A:487:ILE:HD13	1:A:490:MET:HE3	1.92	0.51
1:B:1515:ARG:HD2	1:C:2516:HIS:HB2	1.92	0.51
1:A:311:THR:HA	3:A:3032:HOH:O	2.11	0.51
1:A:487:ILE:HA	1:A:490:MET:CE	2.37	0.50
1:C:2471:GLU:O	1:C:2472:LYS:C	2.50	0.50
1:B:1354:LEU:HD11	1:B:1383:TRP:HB2	1.93	0.50
1:A:531:LYS:O	1:A:533:VAL:HG23	2.12	0.50
1:A:508:LEU:HA	1:A:511:LEU:HG	1.93	0.50
1:B:1466:LEU:O	1:B:1470:GLU:HG3	2.11	0.50
1:C:2451:ILE:HG23	1:C:2479:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2328:TYR:HD2	1:C:2407:ASN:ND2	2.08	0.50
1:C:2497:LEU:HD23	1:C:2500:GLN:NE2	2.25	0.50
1:A:510:ILE:O	1:A:513:HIS:N	2.45	0.50
1:A:328:TYR:HA	1:A:407:ASN:HD21	1.76	0.50
1:C:2361:ALA:CB	1:C:2379:LEU:HD21	2.41	0.50
1:C:2494:GLY:O	1:C:2495:LEU:C	2.50	0.50
1:C:2442:GLY:HA3	3:C:3133:HOH:O	2.11	0.50
1:B:1327:LEU:CG	1:B:1327:LEU:N	2.74	0.50
1:A:391:LEU:CD1	1:A:404:PHE:HA	2.42	0.50
1:B:1514:ILE:HA	1:B:1517:MET:HE3	1.93	0.50
1:B:1433:SER:HA	1:B:1436:ARG:NH2	2.26	0.49
1:B:1471:GLU:O	1:B:1472:LYS:C	2.50	0.49
1:C:2354:LEU:HD11	1:C:2383:TRP:HB2	1.94	0.49
1:A:341:SER:O	1:A:345:LEU:HD23	2.12	0.49
1:C:2463:SER:C	1:C:2468:SER:HB2	2.31	0.49
1:C:2416:LYS:HG2	1:C:2422:VAL:CG2	2.41	0.49
1:C:2409:LEU:HD13	1:C:2410:LEU:N	2.28	0.49
1:B:1448:LEU:HD11	1:B:1507:LEU:CD2	2.41	0.49
1:A:444:GLU:O	1:A:447:CYS:HB2	2.12	0.49
1:C:2536:LEU:HD12	1:C:2536:LEU:N	2.27	0.49
1:C:2382:ALA:HB2	1:C:2456:SER:HB2	1.95	0.49
1:C:2315:MET:O	1:C:2318:ALA:HB3	2.12	0.49
1:A:325:PRO:O	1:A:327:LEU:HD12	2.13	0.49
1:A:343:MET:HE3	1:A:418:VAL:HG11	1.93	0.49
1:B:1436:ARG:C	1:B:1438:MET:H	2.14	0.49
1:A:399:PRO:HB3	1:A:436:ARG:CZ	2.42	0.49
1:B:1366:GLY:HA2	1:B:1369:ASP:OD2	2.12	0.49
1:B:1416:LYS:HG2	1:B:1422:VAL:CG2	2.42	0.49
1:A:358:ILE:HA	1:A:379:LEU:HD11	1.95	0.49
1:A:549:LEU:C	1:A:549:LEU:HD23	2.33	0.49
1:A:466:LEU:HD12	1:A:467:LYS:H	1.76	0.49
1:B:1354:LEU:HD21	1:B:1543:MET:HG3	1.94	0.49
1:C:2433:SER:HA	1:C:2436:ARG:NH2	2.27	0.49
1:B:1405:ALA:HB3	1:B:1408:LEU:HB3	1.95	0.48
1:B:1421:MET:HE3	1:B:1424:ILE:HD12	1.95	0.48
1:C:2327:LEU:HD12	1:C:2352:ARG:NH1	2.27	0.48
1:C:2514:ILE:HA	1:C:2517:MET:HE3	1.94	0.48
1:B:1536:LEU:N	1:B:1536:LEU:HD12	2.27	0.48
1:A:331:TYR:HE1	1:A:337:PHE:CE2	2.31	0.48
1:C:2410:LEU:HD22	1:C:2414:GLN:HG2	1.95	0.48
1:A:421:MET:HA	1:A:421:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:GLU:O	1:B:1547:HIS:HE1	1.95	0.48
1:A:434:ARG:HH22	1:A:506:GLN:HG2	1.78	0.48
1:C:2436:ARG:C	1:C:2438:MET:H	2.16	0.48
1:C:2524:HIS:O	1:C:2527:SER:HB3	2.14	0.48
1:A:424:ILE:O	1:A:427:MET:N	2.46	0.48
1:A:419:GLU:C	1:A:421:MET:N	2.67	0.48
1:B:1510:ILE:O	1:B:1514:ILE:HG13	2.14	0.48
1:A:319:LEU:HD21	1:A:450:SER:HB3	1.94	0.48
1:B:1490:MET:O	1:B:1495:LEU:HB2	2.14	0.48
1:A:427:MET:HE2	1:A:517:MET:HG2	1.95	0.48
1:A:306:LEU:HD21	1:A:310:LEU:HD21	1.96	0.48
1:B:1398:HIS:N	1:B:1398:HIS:ND1	2.60	0.48
1:B:1315:MET:O	1:B:1318:ALA:HB3	2.13	0.47
1:B:1513:HIS:CD2	1:C:2459:TYR:CD1	3.02	0.47
1:C:2401:LYS:HD3	1:C:2409:LEU:CD1	2.44	0.47
1:A:337:PHE:HA	1:A:341:SER:HB3	1.96	0.47
1:B:1491:ALA:C	1:B:1493:ALA:H	2.16	0.47
1:C:2357:MET:CE	1:C:2386:ILE:HB	2.41	0.47
1:A:342:MET:HG2	1:A:346:LEU:HD11	1.97	0.47
1:A:329:SER:C	1:A:331:TYR:N	2.65	0.47
1:A:403:LEU:HD23	1:A:403:LEU:O	2.15	0.47
1:C:2340:ALA:HA	1:C:2533:VAL:HG12	1.96	0.47
1:B:1340:ALA:HA	1:B:1533:VAL:HG12	1.95	0.47
1:C:2496:THR:O	1:C:2499:GLN:N	2.48	0.47
1:C:2392:VAL:HG13	1:C:2432:SER:CA	2.41	0.47
1:A:377:HIS:NE2	1:A:460:THR:O	2.46	0.47
1:A:461:PHE:HD2	1:A:461:PHE:HA	1.63	0.47
1:B:1382:ALA:HB2	1:B:1456:SER:HB2	1.95	0.47
1:C:2398:HIS:ND1	1:C:2398:HIS:N	2.60	0.47
1:A:360:TRP:HA	1:A:363:ARG:CZ	2.44	0.47
1:A:360:TRP:O	1:A:363:ARG:HB2	2.14	0.47
1:A:363:ARG:HD3	3:C:3123:HOH:O	2.13	0.47
1:A:374:ASP:O	1:A:378:LEU:HD12	2.15	0.47
1:C:2366:GLY:HA2	1:C:2369:ASP:OD2	2.15	0.47
1:A:451:ILE:HG13	1:A:482:ILE:HG21	1.95	0.47
1:B:1326:ILE:O	1:B:1327:LEU:CA	2.61	0.47
1:A:374:ASP:O	1:A:377:HIS:HB3	2.15	0.47
1:C:2345:LEU:HD12	1:C:2408:LEU:HD22	1.96	0.46
1:B:1497:LEU:HD23	1:B:1500:GLN:NE2	2.29	0.46
1:C:2423:GLU:H	1:C:2423:GLU:CD	2.18	0.46
1:B:1496:THR:HG23	1:B:1499:GLN:CD	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2472:LYS:HG2	1:C:2476:HIS:CE1	2.51	0.46
1:A:462:LEU:C	1:A:462:LEU:HD12	2.35	0.46
1:C:2304:ASN:HB3	3:C:3140:HOH:O	2.15	0.46
1:A:311:THR:O	1:A:314:GLN:HB2	2.16	0.46
1:C:2428:LEU:HD23	1:C:2517:MET:SD	2.56	0.46
1:C:2354:LEU:HD21	1:C:2543:MET:HG3	1.96	0.46
1:A:490:MET:HG2	3:A:3001:HOH:O	2.14	0.46
1:B:1410:LEU:HD22	1:B:1414:GLN:HG2	1.97	0.46
1:B:1352:ARG:NH1	3:B:3047:HOH:O	2.49	0.46
1:A:334:THR:HG21	3:A:3145:HOH:O	2.15	0.46
1:B:1454:LEU:HB2	1:B:1479:LEU:HD21	1.97	0.46
1:A:318:ALA:HA	1:C:2336:PRO:HG3	1.96	0.46
1:C:2377:HIS:CE1	1:C:2460:THR:O	2.68	0.46
1:A:398:HIS:HE2	1:A:403:LEU:HD12	1.81	0.46
1:B:1459:TYR:HD1	1:C:2513:HIS:CD2	2.33	0.46
1:A:492:LYS:O	1:A:492:LYS:HG2	2.15	0.46
1:A:515:ARG:HG2	3:A:3035:HOH:O	2.15	0.46
1:A:339:GLU:CG	1:A:339:GLU:O	2.55	0.46
1:C:2393:TRP:CH2	1:C:2442:GLY:HA2	2.51	0.46
1:A:411:ASP:OD2	1:A:411:ASP:C	2.54	0.46
1:A:304:ASN:HA	1:A:308:LEU:CD1	2.46	0.46
1:A:328:TYR:C	1:A:407:ASN:HD21	2.20	0.45
1:C:2401:LYS:CD	1:C:2409:LEU:HD11	2.45	0.45
1:A:311:THR:O	1:A:312:ALA:C	2.54	0.45
1:A:445:PHE:CE2	1:A:449:LYS:HD2	2.51	0.45
1:A:328:TYR:CA	1:A:407:ASN:ND2	2.79	0.45
1:A:307:ALA:O	1:A:309:SER:N	2.49	0.45
1:A:508:LEU:O	1:A:511:LEU:HB2	2.16	0.45
1:A:542:GLU:HG2	1:A:543:MET:CE	2.45	0.45
1:A:363:ARG:NE	3:A:3010:HOH:O	2.45	0.45
1:A:388:MET:HG3	2:A:600:EST:H62	1.98	0.45
1:B:1428:LEU:HD23	1:B:1517:MET:SD	2.56	0.45
1:C:2434:ARG:HG2	1:C:2434:ARG:HH11	1.81	0.45
1:C:2306:LEU:HD12	1:C:2306:LEU:C	2.37	0.45
1:B:1393:TRP:CH2	1:B:1442:GLY:HA2	2.51	0.45
1:A:397:GLU:HB3	1:A:398:HIS:CE1	2.52	0.45
1:A:322:ALA:HB1	1:A:363:ARG:HB3	1.99	0.45
1:B:1479:LEU:HA	1:B:1482:ILE:HD12	1.99	0.45
1:B:1451:ILE:HG23	1:B:1479:LEU:HD22	1.97	0.45
1:C:2454:LEU:HB2	1:C:2479:LEU:HD21	1.98	0.45
1:B:1516:HIS:HB2	1:C:2515:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HD22	2:A:600:EST:H183	1.98	0.45
1:B:1361:ALA:CB	1:B:1379:LEU:HD21	2.47	0.45
1:B:1315:MET:CE	1:B:1481:LYS:HG2	2.47	0.45
1:C:2444:GLU:CD	1:C:2503:ARG:HH21	2.20	0.45
1:B:1505:ALA:HA	1:C:2508:LEU:CD1	2.47	0.45
1:A:338:SER:N	1:A:341:SER:HB3	2.28	0.45
1:C:2421:MET:HE3	1:C:2424:ILE:HD12	1.99	0.45
1:C:2372:LEU:HD23	1:C:2375:GLN:NE2	2.32	0.45
1:C:2383:TRP:CG	1:C:2384:LEU:N	2.85	0.45
1:A:413:ASN:O	1:A:414:GLN:C	2.55	0.45
1:B:1434:ARG:HG2	1:B:1434:ARG:HH11	1.81	0.45
1:A:331:TYR:HE1	1:A:337:PHE:HE2	1.65	0.44
1:B:1435:PHE:CE2	1:B:1510:ILE:HG21	2.52	0.44
1:A:536:LEU:HD12	1:A:536:LEU:N	2.32	0.44
1:B:1519:ASN:ND2	1:C:2519:ASN:ND2	2.44	0.44
1:A:529:LYS:C	1:A:531:LYS:N	2.70	0.44
1:C:2454:LEU:HB3	1:C:2475:ILE:HG23	1.99	0.44
1:A:413:ASN:C	1:A:415:GLY:N	2.69	0.44
1:A:549:LEU:O	1:A:550:HIS:ND1	2.50	0.44
1:B:1508:LEU:HD13	1:C:2505:ALA:HA	1.98	0.44
1:B:1515:ARG:CG	1:B:1515:ARG:NH1	2.78	0.44
1:B:1472:LYS:HG2	1:B:1476:HIS:CE1	2.52	0.44
1:B:1383:TRP:CG	1:B:1384:LEU:N	2.85	0.44
1:A:524:HIS:CE1	1:A:528:MET:HG3	2.53	0.44
1:A:388:MET:CE	1:A:517:MET:HB3	2.48	0.44
1:B:1334:THR:O	1:B:1335:ARG:HB2	2.18	0.44
1:A:379:LEU:HD23	1:A:379:LEU:O	2.18	0.44
1:B:1484:ASP:OD2	1:C:2502:GLN:NE2	2.51	0.44
1:C:2307:ALA:HB2	1:C:2366:GLY:N	2.32	0.44
1:C:2416:LYS:HG2	1:C:2422:VAL:HG21	1.99	0.43
1:C:2327:LEU:HD21	1:C:2353:GLU:HB2	2.00	0.43
1:A:403:LEU:CD2	1:A:403:LEU:O	2.66	0.43
1:A:441:GLN:O	1:A:442:GLY:C	2.55	0.43
1:B:1357:MET:CE	1:B:1386:ILE:HB	2.46	0.43
1:A:383:TRP:CD2	1:A:384:LEU:N	2.86	0.43
1:C:2388:MET:HG2	2:C:2600:EST:H62	1.99	0.43
1:A:454:LEU:HD11	1:A:478:VAL:HG11	2.01	0.43
1:B:1472:LYS:HE2	1:B:1476:HIS:HE1	1.84	0.43
1:C:2472:LYS:HE2	1:C:2476:HIS:HE1	1.83	0.43
1:A:485:THR:O	1:A:488:HIS:HB3	2.18	0.43
1:A:545:ASP:O	1:A:548:ARG:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2328:TYR:HD2	1:C:2407:ASN:HD22	1.66	0.43
1:A:537:TYR:O	1:A:538:ASP:C	2.57	0.43
1:C:2490:MET:HE3	1:C:2500:GLN:HB3	2.00	0.43
1:A:466:LEU:CD1	1:A:467:LYS:H	2.30	0.43
1:C:2315:MET:CE	1:C:2481:LYS:HG2	2.45	0.43
1:B:1444:GLU:CD	1:B:1503:ARG:HH21	2.22	0.43
1:A:521:GLY:O	1:A:524:HIS:HB3	2.19	0.43
1:C:2515:ARG:CG	1:C:2515:ARG:NH1	2.80	0.43
1:C:2435:PHE:CE2	1:C:2510:ILE:HG21	2.53	0.43
1:B:1395:SER:O	1:B:1396:MET:C	2.57	0.43
1:A:411:ASP:OD2	1:A:413:ASN:HB2	2.18	0.43
1:C:2328:TYR:HB3	1:C:2407:ASN:ND2	2.24	0.43
1:A:360:TRP:CZ3	1:A:453:LEU:HD22	2.54	0.43
1:B:1372:LEU:HD23	1:B:1375:GLN:NE2	2.33	0.43
1:B:1447:CYS:HB2	1:B:1486:LEU:HD21	2.01	0.43
1:A:326:ILE:HD12	1:A:326:ILE:H	1.83	0.43
1:A:441:GLN:O	1:A:443:GLU:N	2.52	0.43
1:C:2401:LYS:HB3	1:C:2409:LEU:CD1	2.45	0.43
1:C:2346:LEU:HD22	1:C:2404:PHE:CE2	2.54	0.43
1:A:350:ALA:O	1:A:354:LEU:HD13	2.19	0.43
1:B:1490:MET:HE1	1:B:1500:GLN:O	2.19	0.43
1:B:1345:LEU:HD12	1:B:1408:LEU:HD22	2.01	0.43
1:B:1495:LEU:O	1:B:1496:THR:C	2.58	0.43
1:B:1490:MET:HE3	1:B:1500:GLN:HB3	2.01	0.43
1:B:1396:MET:SD	1:B:1435:PHE:HB3	2.59	0.43
1:C:2395:SER:O	1:C:2396:MET:C	2.57	0.43
1:A:389:ILE:HG12	1:A:445:PHE:CE1	2.52	0.43
1:C:2338:SER:N	1:C:2341:SER:HB3	2.33	0.43
1:A:456:SER:HA	1:A:515:ARG:NH2	2.33	0.42
1:B:1466:LEU:N	1:B:1466:LEU:HD22	2.34	0.42
1:C:2463:SER:HB3	1:C:2468:SER:HB2	2.01	0.42
1:B:1401:LYS:HB3	1:B:1409:LEU:CD1	2.47	0.42
1:A:388:MET:HE2	1:A:517:MET:HB3	2.01	0.42
1:B:1487:ILE:HG21	1:C:2501:HIS:ND1	2.34	0.42
1:A:304:ASN:N	3:A:3006:HOH:O	2.52	0.42
1:B:1366:GLY:O	1:B:1474:HIS:HE1	2.02	0.42
1:A:346:LEU:HD22	1:A:404:PHE:CE2	2.54	0.42
1:B:1488:HIS:O	1:B:1490:MET:N	2.52	0.42
1:B:1454:LEU:HB3	1:B:1475:ILE:HG23	2.00	0.42
1:A:399:PRO:HB3	1:A:436:ARG:NH2	2.34	0.42
1:A:443:GLU:O	1:A:446:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1381:CYS:SG	1:B:1457:GLY:HA3	2.59	0.42
1:A:419:GLU:OE1	1:A:531:LYS:NZ	2.53	0.42
1:A:526:TYR:CG	1:A:549:LEU:HD21	2.54	0.42
1:C:2463:SER:O	1:C:2468:SER:OG	2.29	0.42
1:A:331:TYR:HA	1:A:345:LEU:HD11	2.01	0.42
1:A:328:TYR:HA	1:A:407:ASN:ND2	2.34	0.42
1:B:1350:ALA:O	1:B:1351:ASP:C	2.57	0.42
1:A:410:LEU:HD22	1:A:414:GLN:HG2	2.01	0.42
1:A:356:HIS:HB3	3:A:3115:HOH:O	2.19	0.42
1:C:2495:LEU:HA	1:C:2499:GLN:OE1	2.20	0.42
1:A:354:LEU:CD1	1:A:387:LEU:HD11	2.49	0.42
1:A:467:LYS:O	1:A:471:GLU:HG2	2.19	0.42
1:C:2381:CYS:SG	1:C:2457:GLY:HA3	2.60	0.42
1:A:345:LEU:CD2	1:A:345:LEU:H	2.32	0.42
1:A:405:ALA:C	1:A:407:ASN:H	2.23	0.42
1:C:2326:ILE:O	1:C:2327:LEU:C	2.58	0.42
1:A:433:SER:O	1:A:436:ARG:N	2.52	0.42
1:B:1332:ASP:C	1:B:1334:THR:H	2.23	0.42
1:A:534:VAL:O	1:A:534:VAL:CG2	2.67	0.42
1:A:352:ARG:NH2	3:A:3048:HOH:O	2.53	0.42
1:C:2392:VAL:CG1	1:C:2432:SER:HA	2.47	0.42
1:A:461:PHE:HZ	1:A:475:ILE:HD11	1.85	0.42
1:B:1416:LYS:HG2	1:B:1422:VAL:HG21	2.00	0.42
1:A:479:LEU:O	1:A:482:ILE:HB	2.19	0.42
1:A:443:GLU:HB3	1:A:489:LEU:CD1	2.50	0.42
1:B:1397:GLU:O	1:B:1399:PRO:CD	2.68	0.41
1:A:334:THR:CG2	3:A:3145:HOH:O	2.67	0.41
1:C:2479:LEU:HA	1:C:2482:ILE:HD12	2.02	0.41
1:A:327:LEU:CD1	1:A:327:LEU:N	2.84	0.41
1:B:1392:VAL:CG1	1:B:1432:SER:HA	2.44	0.41
1:C:2366:GLY:O	1:C:2474:HIS:HE1	2.03	0.41
1:B:1436:ARG:HG3	3:B:3024:HOH:O	2.20	0.41
1:A:338:SER:H	1:A:341:SER:CB	2.28	0.41
1:A:329:SER:OG	1:A:345:LEU:HD12	2.21	0.41
1:A:458:VAL:HG13	1:A:459:TYR:H	1.85	0.41
1:A:547:HIS:O	1:A:548:ARG:C	2.57	0.41
1:A:331:TYR:CE2	1:A:333:PRO:HB3	2.55	0.41
1:B:1459:TYR:HE2	1:C:2434:ARG:NH1	2.17	0.41
1:A:455:ASN:O	1:A:457:GLY:N	2.54	0.41
1:C:2314:GLN:O	1:C:2318:ALA:HB2	2.20	0.41
1:B:1525:LEU:HD13	2:B:1600:EST:H183	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2490:MET:SD	1:C:2503:ARG:HB3	2.60	0.41
1:A:462:LEU:O	1:A:462:LEU:HD12	2.20	0.41
1:A:316:VAL:O	1:A:317:SER:C	2.59	0.41
1:A:435:PHE:CD1	1:A:440:LEU:HD22	2.56	0.41
1:C:2350:ALA:O	1:C:2351:ASP:C	2.57	0.41
1:B:1403:LEU:HA	1:B:1409:LEU:HD22	2.02	0.41
1:B:1346:LEU:HD22	1:B:1404:PHE:CE2	2.56	0.41
1:A:496:THR:N	1:A:499:GLN:OE1	2.48	0.41
1:B:1401:LYS:HD3	1:B:1409:LEU:CD1	2.48	0.41
1:B:1371:THR:O	1:B:1372:LEU:C	2.59	0.41
1:B:1367:PHE:CZ	1:B:1375:GLN:HB3	2.56	0.41
1:C:2497:LEU:HA	1:C:2500:GLN:NE2	2.36	0.41
1:C:2397:GLU:O	1:C:2399:PRO:CD	2.68	0.41
1:C:2343:MET:SD	1:C:2528:MET:HG3	2.60	0.41
1:C:2462:LEU:HB3	1:C:2463:SER:H	1.69	0.41
1:A:443:GLU:HB3	1:A:489:LEU:HD13	2.03	0.41
1:C:2461:PHE:HA	1:C:2461:PHE:HD2	1.67	0.41
1:C:2319:LEU:HB3	1:C:2446:VAL:HB	2.03	0.41
1:A:391:LEU:CD1	1:A:394:ARG:HH21	2.34	0.40
1:A:427:MET:HE3	1:A:517:MET:HG2	2.00	0.40
1:A:527:SER:O	1:A:531:LYS:HG3	2.21	0.40
1:C:2509:LEU:HA	1:C:2509:LEU:HD23	1.89	0.40
1:A:439:ASN:C	1:A:440:LEU:O	2.58	0.40
1:C:2542:GLU:HG2	1:C:2543:MET:CE	2.51	0.40
1:B:1484:ASP:CG	1:C:2502:GLN:HE21	2.24	0.40
1:A:474:HIS:O	1:A:475:ILE:C	2.58	0.40
1:A:393:TRP:CZ3	1:A:396:MET:HE3	2.57	0.40
1:A:447:CYS:CB	1:A:486:LEU:HD21	2.52	0.40
1:A:422:VAL:O	1:A:423:GLU:C	2.60	0.40
1:A:391:LEU:HD21	1:A:402:LEU:HD22	2.03	0.40
1:B:1338:SER:OG	1:B:1341:SER:CB	2.70	0.40
1:B:1440:LEU:HD13	1:B:1507:LEU:HD21	2.02	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	245/247 (99%)	185 (76%)	43 (18%)	17 (7%)	1	4
1	B	244/247 (99%)	204 (84%)	31 (13%)	9 (4%)	4	17
1	C	242/247 (98%)	202 (84%)	32 (13%)	8 (3%)	5	20
All	All	731/741 (99%)	591 (81%)	106 (14%)	34 (5%)	3	11

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1308	LEU
1	A	306	LEU
1	A	308	LEU
1	A	339	GLU
1	A	403	LEU
1	A	456	SER
1	B	1462	LEU
1	A	307	ALA
1	A	442	GLY
1	A	502	GLN
1	A	538	ASP
1	B	1442	GLY
1	C	2442	GLY
1	A	310	LEU
1	A	330	GLU
1	A	423	GLU
1	C	2336	PRO
1	C	2489	LEU
1	C	2501	HIS
1	A	312	ALA
1	A	440	LEU
1	A	445	PHE
1	B	1396	MET
1	B	1489	LEU
1	C	2327	LEU
1	A	396	MET
1	B	1437	MET
1	B	1501	HIS
1	B	1548	ARG
1	C	2437	MET

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Mol	Chain	Res	Type
1	A	422	VAL
1	C	2326	ILE
1	B	1398	HIS
1	C	2398	HIS

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	223/223 (100%)	197 (88%)	26 (12%)	7	19
1	B	222/223 (100%)	203 (91%)	19 (9%)	13	36
1	C	220/223 (99%)	199 (90%)	21 (10%)	11	31
All	All	665/669 (99%)	599 (90%)	66 (10%)	10	29

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	311	THR
1	A	319	LEU
1	A	332	ASP
1	A	335	ARG
1	A	337	PHE
1	A	379	LEU
1	A	396	MET
1	A	398	HIS
1	A	409	LEU
1	A	422	VAL
1	A	434	ARG
1	A	461	PHE
1	A	462	LEU
1	A	466	LEU
1	A	470	GLU
1	A	492	LYS
1	A	512	SER

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Mol	Chain	Res	Type
1	A	515	ARG
1	A	520	LYS
1	A	532	ASN
1	A	538	ASP
1	A	539	LEU
1	A	541	LEU
1	A	545	ASP
1	A	549	LEU
1	B	1310	LEU
1	B	1326	ILE
1	B	1327	LEU
1	B	1345	LEU
1	B	1374	ASP
1	B	1398	HIS
1	B	1413	ASN
1	B	1414	GLN
1	B	1426	ASP
1	B	1439	ASN
1	B	1461	PHE
1	B	1473	ASP
1	B	1480	ASP
1	B	1489	LEU
1	B	1492	LYS
1	B	1496	THR
1	B	1515	ARG
1	B	1538	ASP
1	B	1541	LEU
1	C	2308	LEU
1	C	2331	TYR
1	C	2345	LEU
1	C	2374	ASP
1	C	2398	HIS
1	C	2413	ASN
1	C	2414	GLN
1	C	2426	ASP
1	C	2439	ASN
1	C	2460	THR
1	C	2461	PHE
1	C	2462	LEU
1	C	2466	LEU
1	C	2473	ASP
1	C	2480	ASP

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Mol	Chain	Res	Type
1	C	2489	LEU
1	C	2492	LYS
1	C	2495	LEU
1	C	2515	ARG
1	C	2538	ASP
1	C	2541	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	359	ASN
1	A	407	ASN
1	A	474	HIS
1	A	506	GLN
1	A	513	HIS
1	B	1314	GLN
1	B	1359	ASN
1	B	1375	GLN
1	B	1439	ASN
1	B	1455	ASN
1	B	1519	ASN
1	B	1547	HIS
1	C	2314	GLN
1	C	2375	GLN
1	C	2439	ASN
1	C	2474	HIS
1	C	2476	HIS
1	C	2500	GLN
1	C	2502	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	EST	A	600	-	23,23,23	2.39	9 (39%)	36,36,36	1.12	3 (8%)
2	EST	B	1600	-	23,23,23	2.47	11 (47%)	36,36,36	1.07	2 (5%)
2	EST	C	2600	-	23,23,23	2.53	9 (39%)	36,36,36	1.04	2 (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	EST	A	600	-	-	0/0/40/40	0/4/4/4
2	EST	B	1600	-	-	0/0/40/40	0/4/4/4
2	EST	C	2600	-	-	0/0/40/40	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1600	EST	C7-C6	2.04	1.56	1.52
2	B	1600	EST	C8-C14	2.08	1.57	1.53
2	B	1600	EST	C18-C13	2.08	1.58	1.54
2	B	1600	EST	C4-C3	2.09	1.42	1.39
2	B	1600	EST	C4-C5	2.21	1.43	1.39
2	A	600	EST	C18-C13	2.24	1.58	1.54
2	A	600	EST	C4-C3	2.32	1.42	1.39
2	C	2600	EST	C4-C5	2.35	1.43	1.39
2	A	600	EST	C7-C6	2.48	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2600	EST	C18-C13	2.78	1.59	1.54
2	B	1600	EST	C2-C1	2.80	1.43	1.38
2	C	2600	EST	C2-C1	2.90	1.44	1.38
2	C	2600	EST	C4-C3	2.91	1.43	1.39
2	A	600	EST	C2-C1	2.99	1.44	1.38
2	A	600	EST	C2-C3	3.10	1.45	1.38
2	B	1600	EST	C10-C9	3.21	1.57	1.52
2	B	1600	EST	C2-C3	3.46	1.45	1.38
2	A	600	EST	C10-C9	3.49	1.57	1.52
2	C	2600	EST	C2-C3	3.59	1.46	1.38
2	C	2600	EST	C10-C9	3.68	1.58	1.52
2	C	2600	EST	C9-C8	3.70	1.58	1.54
2	A	600	EST	C9-C8	4.38	1.59	1.54
2	A	600	EST	C1-C10	4.40	1.45	1.39
2	B	1600	EST	C1-C10	4.74	1.46	1.39
2	A	600	EST	C5-C10	4.99	1.48	1.39
2	C	2600	EST	C1-C10	5.05	1.46	1.39
2	C	2600	EST	C5-C10	5.10	1.48	1.39
2	B	1600	EST	C9-C8	5.12	1.60	1.54
2	B	1600	EST	C5-C10	5.22	1.48	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	EST	C11-C9-C8	-2.48	107.89	111.30
2	C	2600	EST	C11-C9-C8	-2.46	107.92	111.30
2	A	600	EST	C11-C9-C8	-2.40	108.01	111.30
2	C	2600	EST	C6-C7-C8	2.01	113.61	110.67
2	B	1600	EST	C16-C17-C13	2.32	106.39	104.58
2	A	600	EST	C6-C7-C8	2.45	114.27	110.67
2	A	600	EST	C16-C17-C13	2.68	106.66	104.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	EST	2	0
2	B	1600	EST	2	0
2	C	2600	EST	1	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	247/247 (100%)	-0.30	1 (0%)	93	92	19, 45, 78, 98	0
1	B	246/247 (99%)	-0.01	2 (0%)	87	86	46, 70, 85, 95	0
1	C	244/247 (98%)	0.13	8 (3%)	50	42	47, 70, 92, 102	0
All	All	737/741 (99%)	-0.06	11 (1%)	76	74	19, 63, 89, 102	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2334	THR	5.0
1	C	2415	GLY	2.9
1	C	2410	LEU	2.8
1	B	1464	SER	2.5
1	C	2331	TYR	2.5
1	C	2534	VAL	2.4
1	B	1435	PHE	2.1
1	C	2536	LEU	2.1
1	C	2322	ALA	2.0
1	A	462	LEU	2.0
1	C	2421	MET	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.

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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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	EST	A	600	20/20	0.97	0.22	1.48	30,33,35,39	0
2	EST	B	1600	20/20	0.96	0.21	-0.16	34,36,38,39	0
2	EST	C	2600	20/20	0.96	0.19	-0.61	31,36,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.