



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:46 PM GMT

PDB ID : 1QKU
Title : WILD TYPE ESTROGEN NUCLEAR RECEPTOR LIGAND BINDING
DOMAIN COMPLEXED WITH ESTRADIOL
Authors : Ruff, M.; Gangloff, M.; Eiler, S.; Duclaud, S.; Wurtz, J.M.; Moras, D.
Deposited on : 1999-08-05
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

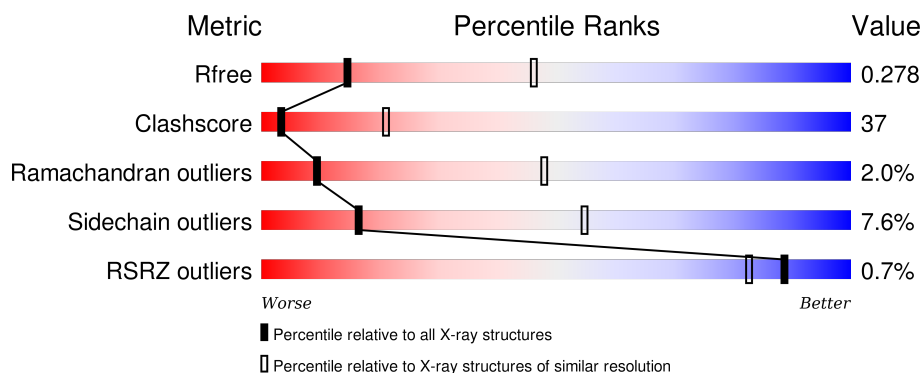
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div></div> <div>53% 43% .</div> </div>
1	B	250	<div> <div></div> <div>42% 51% 6% .</div> </div>
1	C	250	<div> <div></div> <div>45% 48% 6% .</div> </div>

2 Entry composition [i](#)

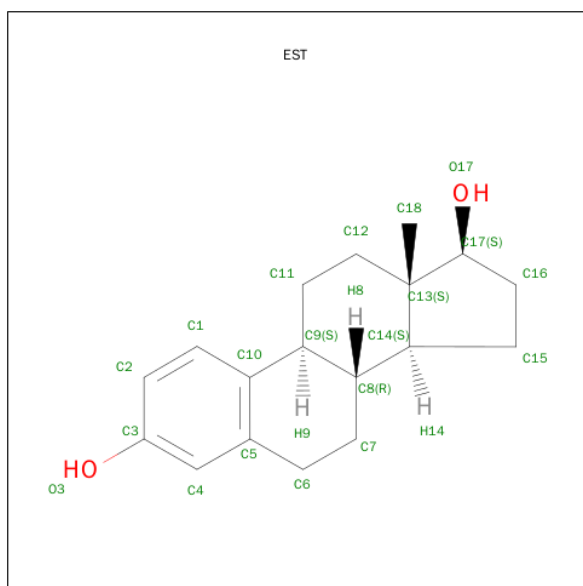
There are 3 unique types of molecules in this entry. The entry contains 6596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ESTRADIOL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1990	1273	341	357	19			
1	B	247	Total	C	N	O	S	0	0	0
			1975	1264	338	354	19			
1	C	247	Total	C	N	O	S	0	0	0
			1975	1264	338	354	19			

- Molecule 2 is ESTRADIOL (three-letter code: EST) (formula: C₁₈H₂₄O₂).



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	177	Total 177	O 177	0	0
3	B	212	Total 212	O 212	0	0
3	C	207	Total 207	O 207	0	0



4 Data and refinement statistics

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)	15.00 – 3.20 49.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.9 (15.00-3.20) 91.0 (49.18-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.91Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.216 , 0.275 0.219 , 0.278	Depositor DCC
R_{free} test set	1357 reflections (9.70%)	DCC
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 18141 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6596	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/2028	0.64	0/2741
1	B	0.43	0/2013	0.64	1/2720 (0.0%)
1	C	0.42	0/2013	0.64	1/2720 (0.0%)
All	All	0.43	0/6054	0.64	2/8181 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	548	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	B	306	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1990	0	2031	120	0
1	B	1975	0	2025	180	0
1	C	1975	0	2025	162	0
2	A	20	0	24	0	0
2	B	20	0	24	0	0
2	C	20	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	177	0	0	16	0
3	B	212	0	0	41	0
3	C	207	0	0	32	0
All	All	6596	0	6153	450	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 37.

All (450) 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:C:549:LEU:O	1:C:549:LEU:HD12	1.28	1.29
1:B:466:LEU:HD11	3:B:2130:HOH:O	1.40	1.19
1:A:548:ARG:HG3	3:A:2169:HOH:O	1.40	1.18
1:C:331:TYR:HA	1:C:345:LEU:HD21	1.34	1.04
1:A:338:SER:H	1:A:341:SER:HB3	1.22	1.02
1:B:392:VAL:HG13	1:B:432:SER:HA	1.40	1.02
1:C:329:SER:H	1:C:407:ASN:HD21	1.00	0.99
1:A:392:VAL:HG13	1:A:432:SER:HA	1.43	0.98
1:A:331:TYR:HB3	1:A:345:LEU:HD21	1.46	0.97
1:C:392:VAL:HG13	1:C:432:SER:HA	1.43	0.95
1:C:549:LEU:O	1:C:549:LEU:CD1	2.16	0.93
1:B:308:LEU:HD21	1:B:477:ARG:CD	2.00	0.91
1:A:329:SER:N	1:A:407:ASN:HD21	1.67	0.91
1:B:515:ARG:HG3	1:B:515:ARG:HH11	1.37	0.88
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.37	0.88
1:B:308:LEU:HD21	1:B:477:ARG:HD3	1.54	0.87
1:B:519:ASN:ND2	1:C:519:ASN:HD22	1.72	0.86
1:A:462:LEU:HB3	3:A:2110:HOH:O	1.74	0.86
1:B:496:THR:HG23	1:B:499:GLN:HG3	1.58	0.86
1:B:519:ASN:HD22	1:C:519:ASN:ND2	1.75	0.85
1:C:515:ARG:HH11	1:C:515:ARG:HG3	1.40	0.83
1:C:329:SER:H	1:C:407:ASN:ND2	1.77	0.82
1:C:455:ASN:HB2	3:C:2117:HOH:O	1.78	0.81
1:C:526:TYR:CG	1:C:549:LEU:HD11	2.15	0.80
1:B:366:GLY:HA2	1:B:369:ASP:OD2	1.81	0.80
1:C:366:GLY:HA2	1:C:369:ASP:OD2	1.82	0.80
1:B:462:LEU:HD12	1:B:463:SER:N	1.97	0.79
1:A:329:SER:H	1:A:407:ASN:HD21	1.27	0.79
1:B:485:THR:HB	3:B:2148:HOH:O	1.83	0.78
1:B:458:VAL:HG21	3:B:2143:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:THR:CG2	1:B:499:GLN:HG3	2.13	0.78
1:B:504:LEU:HD23	1:C:504:LEU:HD23	1.66	0.77
1:A:366:GLY:HA2	1:A:369:ASP:OD2	1.83	0.77
1:B:490:MET:HB2	3:B:2152:HOH:O	1.85	0.77
1:C:304:ASN:N	1:C:308:LEU:HD11	2.01	0.75
1:B:515:ARG:HD2	1:C:516:HIS:HB2	1.67	0.75
1:A:531:LYS:HE3	3:A:2157:HOH:O	1.88	0.74
1:B:463:SER:CB	1:B:468:SER:HB2	2.18	0.74
1:B:519:ASN:HD22	1:C:519:ASN:HD22	1.33	0.73
1:B:328:TYR:HB3	1:B:407:ASN:HD22	1.51	0.73
1:C:526:TYR:CB	1:C:549:LEU:HD11	2.19	0.73
1:C:329:SER:N	1:C:407:ASN:HD21	1.81	0.73
1:C:529:LYS:HA	1:C:534:VAL:HG12	1.69	0.73
1:B:508:LEU:HA	3:B:2176:HOH:O	1.87	0.72
1:C:343:MET:HB3	3:C:2188:HOH:O	1.89	0.72
1:B:305:SER:C	1:B:307:ALA:H	1.92	0.72
1:B:466:LEU:O	1:B:466:LEU:HD22	1.91	0.71
1:B:463:SER:HB2	1:B:468:SER:HB2	1.74	0.70
1:B:519:ASN:ND2	1:C:519:ASN:ND2	2.38	0.70
1:B:529:LYS:HA	1:B:534:VAL:HG12	1.73	0.70
1:A:331:TYR:HB3	1:A:345:LEU:CD2	2.19	0.70
1:B:328:TYR:CE2	1:B:406:PRO:HB2	2.27	0.70
1:B:466:LEU:HD13	1:B:467:LYS:N	2.06	0.69
1:B:338:SER:H	1:B:341:SER:HB3	1.57	0.69
1:B:490:MET:SD	1:B:503:ARG:HD3	2.32	0.69
1:A:529:LYS:HA	1:A:534:VAL:HG12	1.72	0.69
1:C:491:ALA:C	1:C:493:ALA:H	1.96	0.69
1:A:332:ASP:HB3	1:A:335:ARG:HH11	1.58	0.68
1:C:462:LEU:HD12	1:C:463:SER:N	2.07	0.68
1:B:392:VAL:HG13	1:B:432:SER:CA	2.22	0.68
1:B:516:HIS:HB2	1:C:515:ARG:HD2	1.75	0.68
1:C:345:LEU:HD12	1:C:408:LEU:HD22	1.76	0.67
1:C:549:LEU:C	1:C:549:LEU:HD12	2.13	0.67
1:B:549:LEU:HD12	1:B:549:LEU:O	1.94	0.67
1:A:329:SER:OG	1:A:345:LEU:HD11	1.94	0.67
1:A:338:SER:H	1:A:341:SER:CB	2.05	0.66
1:A:549:LEU:HD12	1:A:549:LEU:O	1.95	0.66
1:A:379:LEU:HD12	3:A:2060:HOH:O	1.94	0.66
1:C:396:MET:O	1:C:436:ARG:HD3	1.96	0.66
1:B:496:THR:HG21	3:B:2163:HOH:O	1.94	0.66
1:C:308:LEU:HA	1:C:481:LYS:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:C	1:A:546:ALA:H	1.98	0.65
1:B:396:MET:O	1:B:436:ARG:HD3	1.96	0.65
1:B:491:ALA:C	1:B:493:ALA:H	1.98	0.65
1:C:534:VAL:HA	3:C:2188:HOH:O	1.96	0.65
1:A:345:LEU:HD12	1:A:408:LEU:HD22	1.78	0.65
1:A:515:ARG:CG	1:A:515:ARG:HH11	2.09	0.65
1:A:308:LEU:HD21	1:A:477:ARG:HG2	1.78	0.64
1:B:332:ASP:C	1:B:334:THR:H	2.00	0.64
1:A:329:SER:H	1:A:407:ASN:ND2	1.96	0.64
1:C:343:MET:HE2	3:C:2042:HOH:O	1.96	0.64
1:B:328:TYR:HB3	1:B:407:ASN:ND2	2.13	0.64
1:B:308:LEU:HD21	1:B:477:ARG:HD2	1.81	0.63
1:A:490:MET:HB3	1:A:495:LEU:HD12	1.80	0.63
1:B:327:LEU:O	1:B:327:LEU:HD12	1.99	0.63
1:C:544:LEU:C	1:C:546:ALA:H	2.02	0.63
1:B:544:LEU:C	1:B:546:ALA:H	2.02	0.63
1:C:515:ARG:CG	1:C:515:ARG:HH11	2.13	0.62
1:B:329:SER:HA	1:B:352:ARG:HH22	1.64	0.62
1:B:486:LEU:HG	3:B:2148:HOH:O	1.99	0.62
1:A:396:MET:O	1:A:436:ARG:HD3	1.99	0.62
1:B:345:LEU:HD12	1:B:408:LEU:HD22	1.80	0.61
1:C:544:LEU:HB2	3:C:2195:HOH:O	1.99	0.61
1:C:338:SER:H	1:C:341:SER:HB3	1.63	0.61
1:B:469:LEU:HD11	3:B:2134:HOH:O	2.00	0.61
1:C:418:VAL:HG21	3:C:2042:HOH:O	2.00	0.61
1:C:490:MET:SD	1:C:503:ARG:HD3	2.40	0.61
1:B:371:THR:CG2	1:B:467:LYS:HE2	2.32	0.60
1:B:487:ILE:O	3:B:2152:HOH:O	2.17	0.60
1:A:498:GLN:O	1:A:502:GLN:HG3	2.01	0.60
1:A:515:ARG:NH1	1:A:515:ARG:HG3	2.14	0.60
1:C:312:ALA:HB3	3:C:2008:HOH:O	2.01	0.59
1:C:392:VAL:HG13	1:C:432:SER:CA	2.26	0.59
1:C:351:ASP:OD2	1:C:537:TYR:HB3	2.03	0.59
1:A:462:LEU:HD23	3:A:2110:HOH:O	2.02	0.59
1:A:481:LYS:HB2	3:A:2127:HOH:O	2.03	0.59
1:B:466:LEU:HD13	1:B:466:LEU:C	2.23	0.59
1:A:490:MET:SD	1:A:503:ARG:HD3	2.43	0.59
1:C:529:LYS:HA	1:C:534:VAL:CG1	2.32	0.59
1:A:332:ASP:C	1:A:334:THR:H	2.06	0.58
1:C:373:HIS:HB3	1:C:462:LEU:HD21	1.86	0.58
1:A:463:SER:CB	1:A:468:SER:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ASP:OD2	1:A:537:TYR:HB3	2.04	0.58
1:B:487:ILE:HA	3:B:2152:HOH:O	2.03	0.58
1:A:392:VAL:HG13	1:A:432:SER:CA	2.27	0.58
1:B:515:ARG:HG3	1:B:515:ARG:NH1	2.13	0.57
1:C:311:THR:HA	3:C:2090:HOH:O	2.04	0.57
1:A:332:ASP:OD1	1:A:334:THR:HG23	2.04	0.57
1:C:346:LEU:HD22	1:C:404:PHE:CD2	2.39	0.57
1:C:526:TYR:CD2	1:C:549:LEU:HD11	2.38	0.57
1:C:331:TYR:HA	1:C:345:LEU:CD2	2.20	0.57
1:C:388:MET:HE1	1:C:517:MET:HB3	1.86	0.57
1:B:498:GLN:O	1:B:502:GLN:HG3	2.03	0.57
1:C:311:THR:HG23	1:C:314:GLN:OE1	2.05	0.57
1:B:403:LEU:HG	1:B:409:LEU:HD23	1.86	0.57
1:C:498:GLN:O	1:C:502:GLN:HG3	2.04	0.57
1:B:529:LYS:HA	1:B:534:VAL:CG1	2.35	0.57
1:A:338:SER:N	1:A:341:SER:HB3	2.05	0.56
1:B:508:LEU:HD13	1:C:505:ALA:HA	1.88	0.56
1:A:529:LYS:HA	1:A:534:VAL:CG1	2.35	0.56
1:C:526:TYR:HB2	1:C:549:LEU:HD11	1.87	0.56
1:B:515:ARG:HH11	1:B:515:ARG:CG	2.10	0.56
1:B:351:ASP:OD2	1:B:537:TYR:HB3	2.05	0.56
1:A:403:LEU:HG	1:A:409:LEU:HD23	1.87	0.56
1:B:311:THR:HG23	1:B:314:GLN:OE1	2.05	0.56
1:C:444:GLU:O	1:C:447:CYS:HB2	2.06	0.56
1:C:315:MET:HG2	1:C:485:THR:OG1	2.05	0.56
1:B:346:LEU:HD22	1:B:404:PHE:CD2	2.41	0.56
1:A:461:PHE:HZ	1:A:475:ILE:CD1	2.18	0.55
1:C:451:ILE:HG23	3:C:2117:HOH:O	2.06	0.55
1:B:371:THR:HG21	1:B:467:LYS:HE2	1.88	0.55
1:A:515:ARG:NH1	1:A:515:ARG:CG	2.69	0.55
1:A:463:SER:HB2	1:A:468:SER:HB2	1.88	0.55
3:B:2133:HOH:O	1:C:437:MET:HE2	2.05	0.55
1:A:332:ASP:O	1:A:334:THR:N	2.39	0.55
1:B:460:THR:HA	3:B:2118:HOH:O	2.06	0.55
1:B:410:LEU:HD22	1:B:414:GLN:HG2	1.88	0.55
1:C:345:LEU:CD1	1:C:408:LEU:HD22	2.36	0.55
1:C:346:LEU:HD22	1:C:404:PHE:CE2	2.42	0.55
1:C:392:VAL:HA	3:C:2069:HOH:O	2.07	0.55
1:B:388:MET:CE	1:B:517:MET:HB3	2.37	0.55
1:C:403:LEU:HG	1:C:409:LEU:HD23	1.88	0.54
1:B:371:THR:HG21	1:B:467:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD22	1:A:404:PHE:CD2	2.41	0.54
1:B:437:MET:HE3	3:C:2141:HOH:O	2.06	0.54
1:B:369:ASP:HB2	1:B:474:HIS:CE1	2.43	0.54
1:C:388:MET:CE	1:C:517:MET:HB3	2.37	0.54
1:A:346:LEU:HD22	1:A:404:PHE:CE2	2.43	0.54
1:B:531:LYS:HG3	3:B:2187:HOH:O	2.08	0.54
1:A:444:GLU:O	1:A:447:CYS:HB2	2.08	0.53
1:A:410:LEU:HD22	1:A:414:GLN:HG2	1.89	0.53
1:B:466:LEU:C	1:B:466:LEU:HD22	2.29	0.53
1:B:526:TYR:CB	1:B:549:LEU:HD11	2.39	0.53
1:A:461:PHE:HZ	1:A:475:ILE:HD11	1.73	0.53
1:B:465:THR:O	1:B:468:SER:HB3	2.08	0.53
1:C:346:LEU:HD11	3:C:2103:HOH:O	2.09	0.53
1:C:461:PHE:HB3	3:C:2128:HOH:O	2.08	0.53
1:A:305:SER:OG	1:A:306:LEU:N	2.40	0.53
1:B:437:MET:CE	3:C:2141:HOH:O	2.57	0.53
1:A:369:ASP:HB2	1:A:474:HIS:CE1	2.44	0.53
1:C:398:HIS:N	1:C:398:HIS:ND1	2.57	0.52
1:C:331:TYR:CA	1:C:345:LEU:HD21	2.25	0.52
1:B:463:SER:HB3	1:B:468:SER:HB2	1.91	0.52
1:A:398:HIS:ND1	1:A:398:HIS:N	2.56	0.52
1:C:328:TYR:HD1	1:C:328:TYR:H	1.56	0.52
1:A:332:ASP:CB	1:A:335:ARG:HH11	2.21	0.52
1:C:410:LEU:HD22	1:C:414:GLN:HG2	1.92	0.52
1:B:305:SER:C	1:B:307:ALA:N	2.60	0.52
1:C:345:LEU:HD12	1:C:408:LEU:CD2	2.39	0.52
1:B:525:LEU:HD23	1:B:544:LEU:HD22	1.92	0.52
1:B:388:MET:HE1	1:B:517:MET:HB3	1.92	0.52
1:C:548:ARG:NH2	3:C:2203:HOH:O	2.41	0.52
1:B:444:GLU:O	1:B:447:CYS:HB2	2.09	0.51
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.10	0.51
1:A:312:ALA:HA	3:A:2137:HOH:O	2.10	0.51
1:B:486:LEU:N	3:B:2148:HOH:O	2.42	0.51
1:B:508:LEU:CD1	1:C:505:ALA:HA	2.40	0.51
1:A:403:LEU:HA	1:A:409:LEU:HD22	1.92	0.51
1:B:496:THR:O	1:B:499:GLN:N	2.43	0.51
1:C:369:ASP:HB2	1:C:474:HIS:CE1	2.45	0.51
1:B:398:HIS:N	1:B:398:HIS:ND1	2.58	0.51
1:C:328:TYR:CD1	1:C:328:TYR:N	2.78	0.51
1:A:331:TYR:CB	1:A:345:LEU:HD21	2.29	0.51
1:A:462:LEU:CB	3:A:2110:HOH:O	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:THR:OG1	1:C:314:GLN:HG3	2.10	0.51
1:B:308:LEU:HA	1:B:481:LYS:HE3	1.91	0.51
1:B:364:VAL:HG11	3:B:2113:HOH:O	2.10	0.51
1:B:326:ILE:HG22	1:B:326:ILE:O	2.10	0.51
1:A:538:ASP:N	1:A:538:ASP:OD2	2.43	0.51
1:C:338:SER:O	1:C:339:GLU:C	2.48	0.51
1:C:328:TYR:HD1	1:C:328:TYR:N	2.09	0.51
1:B:515:ARG:NH1	1:B:515:ARG:CG	2.69	0.51
1:B:315:MET:HG2	1:B:485:THR:OG1	2.11	0.50
1:A:311:THR:HG23	1:A:314:GLN:OE1	2.12	0.50
1:B:371:THR:HG21	1:B:467:LYS:CE	2.40	0.50
1:C:515:ARG:NH1	1:C:515:ARG:HG3	2.17	0.50
1:C:380:GLU:O	1:C:547:HIS:CE1	2.65	0.50
1:A:526:TYR:CB	1:A:549:LEU:HD11	2.42	0.50
1:B:330:GLU:O	1:B:330:GLU:CD	2.50	0.50
1:B:403:LEU:HA	1:B:409:LEU:HD22	1.92	0.50
1:C:305:SER:C	1:C:307:ALA:N	2.65	0.50
1:B:453:LEU:HD23	3:B:2113:HOH:O	2.11	0.50
1:B:346:LEU:HD22	1:B:404:PHE:CE2	2.46	0.50
1:A:315:MET:HG2	1:A:485:THR:OG1	2.12	0.50
1:C:406:PRO:HB2	3:C:2076:HOH:O	2.12	0.50
1:B:371:THR:HG21	1:B:467:LYS:HZ3	1.77	0.50
1:B:491:ALA:C	1:B:493:ALA:N	2.65	0.50
1:B:345:LEU:CD1	1:B:408:LEU:HD22	2.42	0.50
1:B:371:THR:CG2	1:B:467:LYS:NZ	2.75	0.49
1:B:331:TYR:CE2	1:B:333:PRO:HG3	2.48	0.49
3:B:2174:HOH:O	1:C:476:HIS:HB3	2.12	0.49
1:C:447:CYS:HB2	1:C:486:LEU:HD21	1.93	0.49
1:C:463:SER:HB3	1:C:465:THR:OG1	2.12	0.49
1:B:337:PHE:CD2	1:B:342:MET:HB2	2.48	0.49
1:B:526:TYR:CG	1:B:549:LEU:HD11	2.48	0.49
1:A:345:LEU:HD12	1:A:408:LEU:CD2	2.43	0.49
1:B:461:PHE:HZ	1:B:475:ILE:HD11	1.78	0.49
1:A:326:ILE:HG22	1:A:326:ILE:O	2.12	0.49
1:A:506:GLN:HG2	3:A:2089:HOH:O	2.12	0.49
1:A:544:LEU:C	1:A:546:ALA:N	2.62	0.49
1:C:422:VAL:HB	1:C:423:GLU:OE1	2.13	0.49
1:C:544:LEU:C	1:C:546:ALA:N	2.64	0.49
1:C:403:LEU:HA	1:C:409:LEU:HD22	1.93	0.48
1:B:538:ASP:N	1:B:538:ASP:OD2	2.46	0.48
1:A:335:ARG:H	1:A:335:ARG:HD2	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HB	1:A:423:GLU:OE1	2.13	0.48
1:A:447:CYS:HB2	1:A:486:LEU:HD21	1.95	0.48
1:A:443:GLU:HB3	1:A:489:LEU:CD1	2.42	0.48
1:A:491:ALA:C	1:A:493:ALA:H	2.16	0.48
1:B:443:GLU:HB3	1:B:489:LEU:CD1	2.43	0.48
1:A:338:SER:O	1:A:339:GLU:C	2.52	0.48
1:A:345:LEU:CD1	1:A:408:LEU:HD22	2.41	0.48
1:B:500:GLN:HB3	3:B:2152:HOH:O	2.13	0.48
1:C:515:ARG:CG	1:C:515:ARG:NH1	2.72	0.48
1:B:332:ASP:O	1:B:334:THR:N	2.46	0.48
1:C:449:LYS:HE2	3:C:2092:HOH:O	2.13	0.48
1:B:523:GLU:HG3	3:B:2182:HOH:O	2.12	0.48
1:B:461:PHE:CZ	1:B:475:ILE:HD11	2.49	0.48
1:C:529:LYS:HB2	1:C:534:VAL:HG11	1.96	0.48
1:C:447:CYS:O	1:C:451:ILE:HG13	2.13	0.48
1:C:403:LEU:HG	1:C:409:LEU:CD2	2.44	0.48
1:C:436:ARG:HA	3:C:2107:HOH:O	2.12	0.48
1:C:460:THR:C	3:C:2121:HOH:O	2.52	0.48
1:C:412:ARG:HB2	3:C:2074:HOH:O	2.13	0.48
1:A:332:ASP:HB2	3:A:2037:HOH:O	2.14	0.48
1:B:447:CYS:HB2	1:B:486:LEU:HD21	1.95	0.48
1:C:491:ALA:C	1:C:493:ALA:N	2.65	0.48
1:C:538:ASP:OD2	1:C:538:ASP:N	2.45	0.48
1:B:509:LEU:HD13	3:C:2117:HOH:O	2.14	0.47
1:A:311:THR:OG1	1:A:314:GLN:HG3	2.14	0.47
1:A:352:ARG:HD2	3:A:2047:HOH:O	2.14	0.47
1:B:308:LEU:HB2	3:B:2006:HOH:O	2.14	0.47
1:B:477:ARG:HD2	3:B:2003:HOH:O	2.14	0.47
1:B:345:LEU:HD12	1:B:408:LEU:CD2	2.44	0.47
1:A:388:MET:CE	1:A:517:MET:HB3	2.44	0.47
1:B:338:SER:O	1:B:339:GLU:C	2.50	0.47
1:B:544:LEU:C	1:B:546:ALA:N	2.64	0.47
1:B:403:LEU:HG	1:B:409:LEU:CD2	2.44	0.47
1:C:443:GLU:HB3	1:C:489:LEU:CD1	2.45	0.47
1:C:418:VAL:HB	1:C:421:MET:HB2	1.96	0.47
1:B:534:VAL:HG22	1:B:535:PRO:O	2.15	0.47
1:C:531:LYS:HB2	3:C:2101:HOH:O	2.14	0.47
1:C:354:LEU:HD21	1:C:543:MET:HG3	1.96	0.47
1:A:526:TYR:CG	1:A:549:LEU:HD11	2.48	0.47
1:C:423:GLU:H	1:C:423:GLU:CD	2.18	0.47
1:B:526:TYR:HB2	1:B:549:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:C	1:A:549:LEU:HD12	2.34	0.47
1:B:418:VAL:HB	1:B:421:MET:HB2	1.97	0.46
1:B:329:SER:N	1:B:407:ASN:HD21	2.13	0.46
1:B:310:LEU:HD22	1:B:314:GLN:HB3	1.98	0.46
1:B:466:LEU:HD23	3:B:2135:HOH:O	2.15	0.46
1:B:305:SER:O	1:B:307:ALA:N	2.48	0.46
1:A:343:MET:CE	1:A:343:MET:HA	2.46	0.46
1:B:392:VAL:HG11	1:B:431:THR:HG22	1.96	0.46
1:A:534:VAL:HG22	1:A:535:PRO:O	2.15	0.46
1:B:422:VAL:HB	1:B:423:GLU:OE1	2.16	0.46
1:B:454:LEU:HB2	1:B:479:LEU:HD21	1.96	0.46
1:A:392:VAL:HG11	1:A:431:THR:HG22	1.98	0.46
1:B:495:LEU:O	1:B:496:THR:C	2.54	0.46
1:A:403:LEU:HG	1:A:409:LEU:CD2	2.45	0.46
1:A:413:ASN:O	1:A:414:GLN:C	2.52	0.46
1:A:418:VAL:HB	1:A:421:MET:HB2	1.98	0.46
1:C:331:TYR:HB3	1:C:345:LEU:HD11	1.98	0.46
1:C:523:GLU:HG3	3:C:2174:HOH:O	2.14	0.46
1:B:453:LEU:HB3	3:B:2113:HOH:O	2.15	0.46
1:A:354:LEU:HD21	1:A:543:MET:HG3	1.98	0.46
1:C:479:LEU:HD13	3:C:2117:HOH:O	2.16	0.46
1:B:397:GLU:HG2	3:B:2120:HOH:O	2.16	0.46
1:C:305:SER:O	1:C:307:ALA:N	2.49	0.45
1:C:359:ASN:N	1:C:359:ASN:HD22	2.14	0.45
1:B:496:THR:O	1:B:497:LEU:C	2.55	0.45
1:C:542:GLU:HG2	1:C:543:MET:CE	2.47	0.45
1:C:306:LEU:HA	1:C:309:SER:OG	2.15	0.45
1:B:536:LEU:HD12	1:B:536:LEU:H	1.82	0.45
1:B:357:MET:HE3	3:B:2042:HOH:O	2.17	0.45
1:C:310:LEU:HD22	1:C:314:GLN:HB3	1.97	0.45
1:A:310:LEU:HD22	1:A:314:GLN:HB3	1.98	0.45
1:A:383:TRP:CG	1:A:384:LEU:N	2.83	0.45
1:B:332:ASP:C	1:B:334:THR:N	2.70	0.45
1:B:515:ARG:CD	1:C:516:HIS:HB2	2.42	0.45
1:B:354:LEU:HD11	1:B:383:TRP:HB2	1.99	0.45
1:B:371:THR:CG2	1:B:467:LYS:CE	2.95	0.45
1:C:308:LEU:CA	1:C:481:LYS:HE3	2.45	0.45
1:C:308:LEU:C	1:C:481:LYS:HE3	2.38	0.45
1:B:511:LEU:HG	3:B:2176:HOH:O	2.17	0.45
1:B:308:LEU:CD2	1:B:477:ARG:HD3	2.38	0.45
1:A:423:GLU:CD	1:A:423:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASN:O	1:B:414:GLN:C	2.55	0.44
1:B:536:LEU:HD12	1:B:536:LEU:N	2.32	0.44
1:B:539:LEU:HB2	3:B:2200:HOH:O	2.17	0.44
1:B:315:MET:O	1:B:319:LEU:HG	2.17	0.44
1:A:454:LEU:HD22	1:A:475:ILE:HG23	1.99	0.44
1:C:447:CYS:CB	1:C:486:LEU:HD21	2.47	0.44
1:A:525:LEU:HD23	1:A:544:LEU:HD22	1.99	0.44
1:C:340:ALA:HA	1:C:533:VAL:CG1	2.48	0.44
1:A:464:SER:CB	3:A:2111:HOH:O	2.65	0.44
1:C:526:TYR:CG	1:C:549:LEU:CD1	2.95	0.44
1:C:308:LEU:HA	1:C:481:LYS:CE	2.46	0.44
1:A:413:ASN:O	1:A:416:LYS:N	2.43	0.44
1:A:329:SER:HB3	1:A:407:ASN:OD1	2.17	0.44
1:C:466:LEU:HD13	1:C:467:LYS:N	2.32	0.44
1:B:383:TRP:CG	1:B:384:LEU:N	2.86	0.44
1:A:513:HIS:O	1:A:516:HIS:HB3	2.17	0.44
1:C:342:MET:HG2	3:C:2042:HOH:O	2.18	0.44
1:B:469:LEU:O	1:B:473:ASP:HB2	2.18	0.44
1:A:496:THR:HG23	1:A:499:GLN:OE1	2.17	0.44
1:C:368:VAL:HG22	3:C:2060:HOH:O	2.18	0.44
1:C:328:TYR:HB3	1:C:407:ASN:HD22	1.83	0.43
1:B:462:LEU:C	1:B:462:LEU:HD12	2.39	0.43
1:B:475:ILE:HG12	3:B:2140:HOH:O	2.18	0.43
1:C:343:MET:CE	1:C:343:MET:HA	2.47	0.43
1:C:490:MET:SD	1:C:503:ARG:HB3	2.59	0.43
1:B:354:LEU:HD21	1:B:543:MET:HG3	2.00	0.43
1:C:418:VAL:HB	1:C:421:MET:CB	2.48	0.43
1:B:522:MET:HG2	1:B:549:LEU:HD23	2.00	0.43
1:B:413:ASN:O	1:B:416:LYS:N	2.47	0.43
1:C:305:SER:C	1:C:307:ALA:H	2.21	0.43
1:C:354:LEU:HD11	1:C:383:TRP:HB2	2.00	0.43
1:A:542:GLU:HG2	1:A:543:MET:CE	2.48	0.43
1:B:513:HIS:O	1:B:516:HIS:HB3	2.19	0.43
1:C:529:LYS:HB2	3:C:2176:HOH:O	2.18	0.43
1:C:536:LEU:N	1:C:536:LEU:HD12	2.33	0.43
1:A:463:SER:HB3	1:A:468:SER:HB2	1.99	0.43
1:C:454:LEU:HB2	1:C:479:LEU:HD21	2.01	0.43
1:C:534:VAL:HG22	1:C:535:PRO:O	2.18	0.43
1:A:308:LEU:CD2	1:A:477:ARG:HG2	2.45	0.43
1:C:315:MET:O	1:C:318:ALA:HB3	2.18	0.43
1:A:315:MET:O	1:A:319:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LEU:H	1:C:536:LEU:HD12	1.82	0.43
1:C:495:LEU:HG	1:C:499:GLN:HB3	2.00	0.43
1:B:459:TYR:HE2	1:C:434:ARG:HH11	1.66	0.43
1:B:327:LEU:HD21	1:B:353:GLU:HA	2.01	0.43
1:A:443:GLU:HB3	1:A:489:LEU:HD11	2.01	0.43
1:B:448:LEU:CD2	3:B:2176:HOH:O	2.66	0.43
1:B:448:LEU:HD22	3:B:2176:HOH:O	2.19	0.43
1:A:335:ARG:HG2	1:A:335:ARG:O	2.19	0.43
1:C:517:MET:HB2	1:C:517:MET:HE2	1.90	0.43
1:A:418:VAL:HB	1:A:421:MET:CB	2.49	0.43
1:B:308:LEU:CA	1:B:481:LYS:HE3	2.49	0.43
1:C:461:PHE:CZ	1:C:475:ILE:HD11	2.54	0.43
1:C:380:GLU:O	1:C:547:HIS:HE1	2.02	0.43
1:C:392:VAL:HG11	1:C:431:THR:HG22	2.00	0.43
3:B:2133:HOH:O	1:C:434:ARG:HA	2.19	0.42
1:B:418:VAL:HB	1:B:421:MET:CB	2.49	0.42
1:B:419:GLU:HB2	3:B:2091:HOH:O	2.19	0.42
1:B:365:PRO:HA	3:B:2053:HOH:O	2.18	0.42
1:C:332:ASP:O	1:C:332:ASP:OD1	2.37	0.42
1:B:449:LYS:HE2	3:B:2018:HOH:O	2.17	0.42
1:B:490:MET:SD	1:B:503:ARG:HB3	2.59	0.42
1:C:501:HIS:O	1:C:504:LEU:HB3	2.20	0.42
1:B:331:TYR:HB2	1:B:345:LEU:HD11	2.01	0.42
1:B:501:HIS:CD2	1:C:501:HIS:CD2	3.06	0.42
1:B:497:LEU:HA	1:B:500:GLN:NE2	2.34	0.42
1:C:525:LEU:HD23	1:C:544:LEU:HD22	2.00	0.42
1:C:469:LEU:O	1:C:473:ASP:HB2	2.18	0.42
1:C:413:ASN:O	1:C:416:LYS:N	2.46	0.42
1:B:423:GLU:CD	1:B:423:GLU:H	2.21	0.42
1:C:470:GLU:HA	3:C:2136:HOH:O	2.18	0.42
1:B:461:PHE:HD2	1:B:461:PHE:HA	1.68	0.42
1:C:411:ASP:OD2	1:C:414:GLN:OE1	2.36	0.42
1:B:367:PHE:CE2	1:B:375:GLN:HB3	2.55	0.42
1:B:343:MET:CE	1:B:343:MET:HA	2.49	0.42
1:B:490:MET:HE3	3:B:2152:HOH:O	2.18	0.42
1:C:315:MET:O	1:C:319:LEU:HG	2.18	0.42
1:A:466:LEU:HD13	1:A:466:LEU:C	2.39	0.42
1:A:447:CYS:CB	1:A:486:LEU:HD21	2.49	0.42
1:A:388:MET:HE1	1:A:517:MET:HB3	2.01	0.42
1:C:352:ARG:HD3	3:C:2048:HOH:O	2.18	0.42
1:B:468:SER:HA	3:B:2059:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:HIS:O	1:B:504:LEU:HB3	2.20	0.42
1:A:536:LEU:H	1:A:536:LEU:HD12	1.85	0.42
1:C:497:LEU:HA	1:C:500:GLN:NE2	2.35	0.42
1:B:308:LEU:C	1:B:481:LYS:HE3	2.40	0.41
1:C:451:ILE:CG1	1:C:482:ILE:HG21	2.50	0.41
3:B:2178:HOH:O	1:C:460:THR:HG23	2.19	0.41
1:C:383:TRP:CG	1:C:384:LEU:N	2.88	0.41
1:A:497:LEU:HA	1:A:500:GLN:NE2	2.35	0.41
1:A:396:MET:HE3	3:A:2093:HOH:O	2.20	0.41
1:B:419:GLU:C	1:B:421:MET:H	2.23	0.41
1:C:523:GLU:OE2	1:C:549:LEU:HB2	2.21	0.41
1:A:454:LEU:HB2	1:A:479:LEU:HD21	2.01	0.41
1:C:549:LEU:O	1:C:549:LEU:CG	2.67	0.41
1:C:343:MET:SD	1:C:528:MET:HG3	2.60	0.41
1:C:439:ASN:HA	3:C:2107:HOH:O	2.20	0.41
1:B:529:LYS:HB2	1:B:534:VAL:HG11	2.03	0.41
1:A:419:GLU:C	1:A:421:MET:H	2.23	0.41
1:B:540:LEU:HD23	3:B:2196:HOH:O	2.20	0.41
1:A:526:TYR:HB2	1:A:549:LEU:HD11	2.03	0.41
1:B:416:LYS:HA	1:B:422:VAL:HG22	2.03	0.41
1:A:311:THR:HA	3:A:2015:HOH:O	2.19	0.41
1:A:536:LEU:HD12	1:A:536:LEU:N	2.34	0.41
1:C:345:LEU:HD13	3:C:2024:HOH:O	2.21	0.41
1:C:487:ILE:HD13	1:C:490:MET:HE3	2.02	0.41
1:B:443:GLU:HB3	1:B:489:LEU:HD11	2.03	0.41
1:A:514:ILE:HA	1:A:517:MET:HE2	2.03	0.41
1:A:309:SER:N	3:A:2013:HOH:O	2.53	0.41
1:B:458:VAL:HG23	1:B:475:ILE:HD12	2.03	0.41
1:C:465:THR:HB	1:C:466:LEU:H	1.65	0.41
1:A:371:THR:OG1	1:A:374:ASP:OD2	2.39	0.41
1:C:329:SER:HB2	3:C:2024:HOH:O	2.21	0.40
1:A:462:LEU:CG	1:A:463:SER:N	2.84	0.40
1:A:469:LEU:O	1:A:473:ASP:HB2	2.21	0.40
1:B:340:ALA:HA	1:B:533:VAL:CG1	2.50	0.40
1:B:508:LEU:CA	3:B:2176:HOH:O	2.60	0.40
1:C:463:SER:HB2	1:C:468:SER:HB2	2.03	0.40
1:C:525:LEU:HD13	2:C:600:EST:H183	2.04	0.40
1:B:310:LEU:HD22	1:B:314:GLN:CB	2.51	0.40
1:B:399:PRO:HD2	3:B:2067:HOH:O	2.22	0.40
1:B:507:LEU:C	3:B:2176:HOH:O	2.60	0.40
1:C:306:LEU:O	1:C:310:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:VAL:HG23	1:C:475:ILE:HD12	2.02	0.40
1:C:542:GLU:HG2	1:C:543:MET:HE3	2.03	0.40
1:A:327:LEU:N	1:A:327:LEU:HD12	2.37	0.40
1:A:316:VAL:C	1:A:318:ALA:N	2.73	0.40
1:B:447:CYS:O	1:B:451:ILE:HG13	2.20	0.40
1:A:529:LYS:HB2	1:A:534:VAL:HG11	2.03	0.40
1:A:487:ILE:HD13	1:A:490:MET:HE3	2.04	0.40
1:B:359:ASN:HD22	1:B:359:ASN:N	2.17	0.40
1:B:447:CYS:CB	1:B:486:LEU:HD21	2.51	0.40
1:A:436:ARG:HG3	3:A:2070:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	248/250 (99%)	215 (87%)	29 (12%)	4 (2%)	12	54
1	B	245/250 (98%)	213 (87%)	26 (11%)	6 (2%)	7	43
1	C	245/250 (98%)	208 (85%)	32 (13%)	5 (2%)	9	48
All	All	738/750 (98%)	636 (86%)	87 (12%)	15 (2%)	9	48

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	327	LEU
1	B	306	LEU
1	B	492	LYS
1	C	306	LEU
1	C	334	THR
1	A	327	LEU
1	A	333	PRO

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Mol	Chain	Res	Type
1	B	333	PRO
1	C	492	LYS
1	A	310	LEU
1	B	442	GLY
1	A	442	GLY
1	C	494	GLY
1	B	326	ILE
1	C	442	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/226 (99%)	207 (93%)	16 (7%)	18	57
1	B	223/226 (99%)	206 (92%)	17 (8%)	16	55
1	C	223/226 (99%)	205 (92%)	18 (8%)	15	51
All	All	669/678 (99%)	618 (92%)	51 (8%)	16	55

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	320	LEU
1	A	330	GLU
1	A	331	TYR
1	A	335	ARG
1	A	345	LEU
1	A	379	LEU
1	A	396	MET
1	A	398	HIS
1	A	409	LEU
1	A	439	ASN
1	A	473	ASP
1	A	492	LYS
1	A	515	ARG

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Mol	Chain	Res	Type
1	A	539	LEU
1	A	541	LEU
1	B	320	LEU
1	B	327	LEU
1	B	329	SER
1	B	335	ARG
1	B	345	LEU
1	B	379	LEU
1	B	396	MET
1	B	398	HIS
1	B	409	LEU
1	B	439	ASN
1	B	466	LEU
1	B	473	ASP
1	B	492	LYS
1	B	496	THR
1	B	515	ARG
1	B	539	LEU
1	B	541	LEU
1	C	308	LEU
1	C	320	LEU
1	C	328	TYR
1	C	331	TYR
1	C	345	LEU
1	C	379	LEU
1	C	396	MET
1	C	398	HIS
1	C	409	LEU
1	C	439	ASN
1	C	461	PHE
1	C	466	LEU
1	C	473	ASP
1	C	492	LYS
1	C	495	LEU
1	C	515	ARG
1	C	539	LEU
1	C	541	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	407	ASN
1	A	439	ASN
1	A	474	HIS
1	A	500	GLN
1	B	348	ASN
1	B	356	HIS
1	B	359	ASN
1	B	407	ASN
1	B	439	ASN
1	B	519	ASN
1	B	550	HIS
1	C	304	ASN
1	C	348	ASN
1	C	356	HIS
1	C	359	ASN
1	C	407	ASN
1	C	439	ASN
1	C	474	HIS
1	C	500	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.66	5 (21%)	36,36,36	1.14	5 (13%)
2	EST	B	600	-	23,23,23	1.64	5 (21%)	36,36,36	1.07	5 (13%)
2	EST	C	600	-	23,23,23	1.81	6 (26%)	36,36,36	1.04	4 (11%)

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	600	-	-	0/0/40/40	0/4/4/4
2	EST	C	600	-	-	0/0/40/40	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	EST	C8-C14	2.08	1.57	1.53
2	A	600	EST	C1-C10	2.15	1.42	1.39
2	C	600	EST	C4-C5	2.16	1.43	1.39
2	B	600	EST	C4-C5	2.21	1.43	1.39
2	A	600	EST	C4-C5	2.25	1.43	1.39
2	C	600	EST	C18-C13	2.26	1.58	1.54
2	C	600	EST	C10-C9	2.28	1.55	1.52
2	A	600	EST	C8-C14	2.29	1.58	1.53
2	C	600	EST	C4-C3	2.63	1.43	1.39
2	B	600	EST	C9-C8	2.64	1.57	1.54
2	B	600	EST	C1-C10	2.79	1.43	1.39
2	A	600	EST	C9-C8	2.80	1.57	1.54
2	A	600	EST	C5-C10	3.04	1.45	1.39
2	C	600	EST	C5-C10	3.50	1.45	1.39
2	C	600	EST	C1-C10	3.54	1.44	1.39
2	B	600	EST	C5-C10	3.66	1.46	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	EST	C11-C9-C8	-2.75	107.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	EST	C15-C14-C13	-2.66	100.36	103.82
2	B	600	EST	C15-C14-C13	-2.60	100.44	103.82
2	C	600	EST	C15-C14-C13	-2.40	100.69	103.82
2	B	600	EST	C11-C9-C8	-2.24	108.23	111.30
2	C	600	EST	C11-C9-C8	-2.06	108.47	111.30
2	B	600	EST	C16-C17-C13	2.02	106.15	104.58
2	A	600	EST	C16-C17-C13	2.04	106.17	104.58
2	A	600	EST	C6-C7-C8	2.06	113.69	110.67
2	B	600	EST	C12-C11-C9	2.14	114.70	112.20
2	C	600	EST	C6-C7-C8	2.18	113.86	110.67
2	B	600	EST	C6-C7-C8	2.19	113.89	110.67
2	C	600	EST	C12-C11-C9	2.34	114.93	112.20
2	A	600	EST	C12-C11-C9	2.76	115.42	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	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	250/250 (100%)	-0.43	2 (0%) 87 80	23, 51, 85, 107	0
1	B	247/250 (98%)	-0.47	1 (0%) 93 90	30, 56, 79, 112	0
1	C	247/250 (98%)	-0.30	2 (0%) 87 80	31, 58, 89, 101	0
All	All	744/750 (99%)	-0.40	5 (0%) 89 83	23, 55, 86, 112	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	SER	4.0
1	A	462	LEU	3.4
1	B	464	SER	3.3
1	C	536	LEU	2.2
1	C	549	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 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, 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(\AA^2)	Q<0.9
2	EST	A	600	20/20	0.97	0.20	0.81	19,23,27,31	0
2	EST	B	600	20/20	0.96	0.18	-0.28	21,25,28,30	0
2	EST	C	600	20/20	0.97	0.18	-0.58	21,26,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.