Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:12 PM GMT

PDB ID	:	1SMS
Title	:	Structure of the Ribonucleotide Reductase Rnr4 Homodimer from Saccharomyces cerevisiae
Authors	:	Sommerhalter, M.; Voegtli, W.C.; Perlstein, D.L.; Ge, J.; Stubbe, J.; Rosenzweig, A.C.
Deposited on	:	2004-03-09
Resolution	:	3.10 Å(reported)

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

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

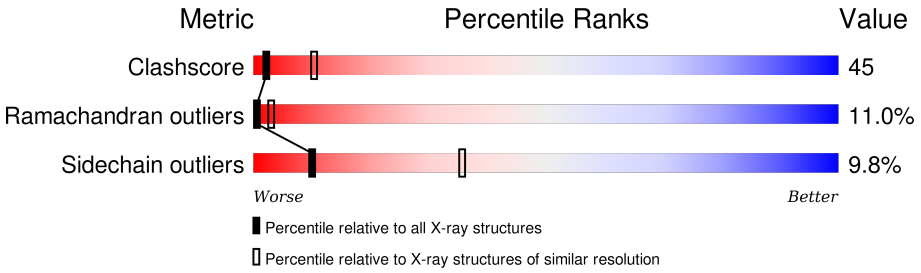
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	27% 52% 10% • 9%
1	B	345	27% 52% 10% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5182 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 Ribonucleoside-diphosphate reductase small chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2589	1679	416	480	14			
1	B	314	Total	C	N	O	S	0	0	0
			2589	1679	416	480	14			

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Hg	0	0
			2	2		
2	A	2	Total	Hg	0	0
			2	2		

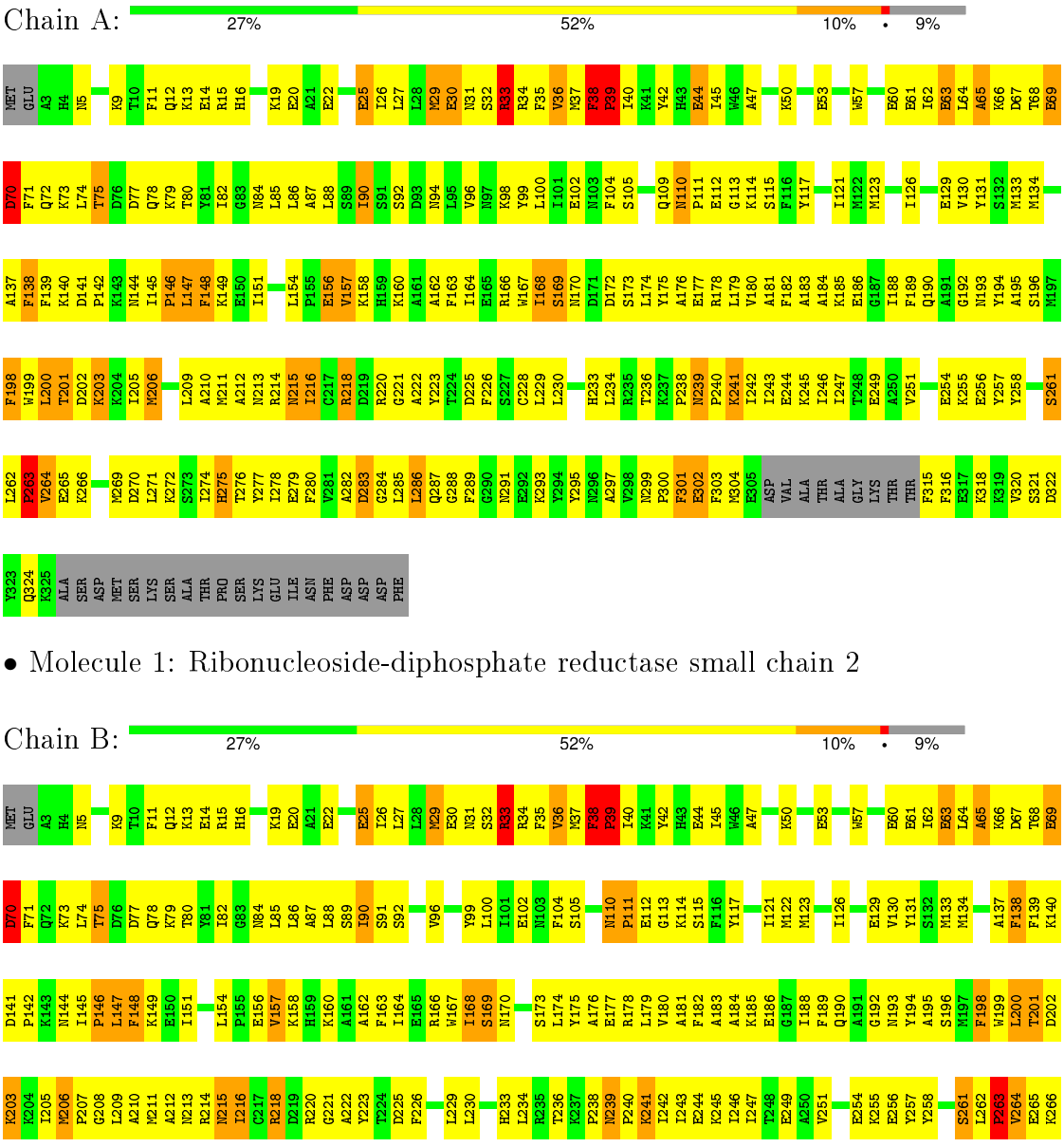
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

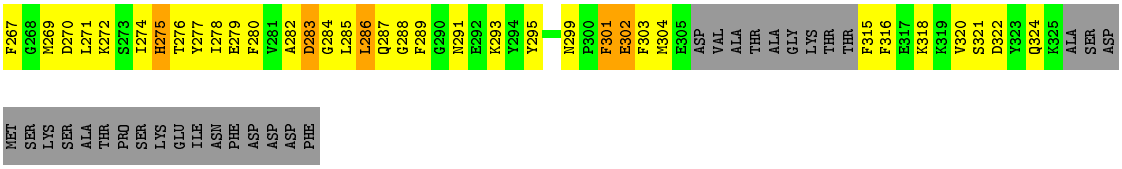
- Molecule 1: Ribonucleoside-diphosphate reductase small chain 2

Chain A:



- Molecule 1: Ribonucleoside-diphosphate reductase small chain 2

Chain B:


F267 G268 M269 D270 L271 K272 S273 I274 H275 T276 Y277 I278 E279 F280 Y281 A282 D283 G284 L285 L286 Q287 G288 F289 G290 N291 E292 K293 Y294 Y295 N299 P300 F301 E302 F303 M304 E305 ASP VAL ALA THR ALA GLY LYS THR THR F315 F316 E317 K318 K319 V320 S321 D322 Y323 Q324 K325 ALA SER ASP
MET SER LYS SER ALA THR PRO SER LYS GLU ILE ASN PHE ASP ASP ASP PHE

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	79.60Å 79.60Å 218.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.266 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5182	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.44	0/2652	0.66	2/3569 (0.1%)
1	B	0.43	0/2652	0.66	2/3569 (0.1%)
All	All	0.43	0/5304	0.66	4/7138 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	MET	N-CA-C	-6.42	93.67	111.00
1	A	37	MET	N-CA-C	-6.39	93.73	111.00
1	A	302	GLU	CB-CA-C	5.33	121.05	110.40
1	B	302	GLU	CB-CA-C	5.32	121.03	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	0	2530	232	0
1	B	2589	0	2530	230	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	5182	0	5060	456	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 45.

All (456) 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:147:LEU:HD11	1:B:154:LEU:HD11	1.34	1.07
1:A:147:LEU:HD11	1:A:154:LEU:HD11	1.34	1.04
1:A:26:ILE:HA	1:A:29:MET:HB2	1.44	0.99
1:B:26:ILE:HA	1:B:29:MET:HB2	1.44	0.97
1:A:239:ASN:ND2	1:A:241:LYS:H	1.68	0.91
1:B:239:ASN:ND2	1:B:241:LYS:H	1.69	0.90
1:A:239:ASN:HD22	1:A:240:PRO:N	1.72	0.88
1:B:88:LEU:O	1:B:92:SER:HB3	1.73	0.87
1:B:239:ASN:HD22	1:B:240:PRO:N	1.72	0.86
1:A:88:LEU:O	1:A:92:SER:HB3	1.75	0.83
1:B:239:ASN:C	1:B:239:ASN:HD22	1.82	0.82
1:A:239:ASN:HD22	1:A:239:ASN:C	1.83	0.80
1:A:316:PHE:O	1:A:320:VAL:HG23	1.81	0.79
1:A:195:ALA:HA	1:A:303:PHE:HZ	1.46	0.79
1:B:316:PHE:O	1:B:320:VAL:HG23	1.83	0.78
1:B:195:ALA:HA	1:B:303:PHE:HZ	1.47	0.77
1:B:74:LEU:HD22	1:B:78:GLN:OE1	1.86	0.76
1:A:202:ASP:OD1	1:A:203:LYS:HG3	1.86	0.75
1:B:202:ASP:OD1	1:B:203:LYS:HG3	1.85	0.74
1:A:74:LEU:HD22	1:A:78:GLN:OE1	1.88	0.73
1:A:321:SER:HA	1:A:324:GLN:HG3	1.72	0.72
1:B:145:ILE:HG22	1:B:148:PHE:HB2	1.72	0.72
1:A:234:LEU:H	1:A:234:LEU:HD12	1.56	0.71
1:A:216:ILE:HG23	1:A:220:ARG:NH2	2.06	0.71
1:B:234:LEU:HD12	1:B:234:LEU:H	1.55	0.71
1:B:185:LYS:HA	1:B:189:PHE:HD2	1.56	0.70
1:A:145:ILE:HG22	1:A:148:PHE:HB2	1.72	0.70
1:B:321:SER:HA	1:B:324:GLN:HG3	1.73	0.70
1:B:38:PHE:O	1:B:39:PRO:C	2.31	0.69
1:A:185:LYS:HA	1:A:189:PHE:HD2	1.57	0.69
1:B:185:LYS:HA	1:B:189:PHE:CD2	2.28	0.69
1:B:112:GLU:O	1:B:115:SER:HB2	1.92	0.69
1:B:283:ASP:OD2	1:B:293:LYS:HB3	1.93	0.69
1:A:185:LYS:HA	1:A:189:PHE:CD2	2.28	0.68
1:A:112:GLU:O	1:A:115:SER:HB2	1.94	0.68
1:B:216:ILE:HG23	1:B:220:ARG:NH2	2.08	0.68
1:B:151:ILE:HA	1:B:154:LEU:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:SER:HA	1:A:324:GLN:CG	2.24	0.67
1:A:254:GLU:HG3	1:A:278:ILE:HD13	1.75	0.67
1:B:211:MET:HA	1:B:214:ARG:NH1	2.10	0.67
1:A:38:PHE:O	1:A:39:PRO:C	2.32	0.67
1:B:145:ILE:CG2	1:B:148:PHE:HB2	2.25	0.67
1:B:321:SER:HA	1:B:324:GLN:CG	2.25	0.67
1:A:188:ILE:CD1	1:A:247:ILE:HG23	2.25	0.66
1:A:38:PHE:HB3	1:A:39:PRO:HD3	1.77	0.66
1:B:245:LYS:HB3	1:B:245:LYS:HZ2	1.59	0.66
1:B:57:TRP:HB2	1:B:61:GLU:OE2	1.96	0.66
1:B:188:ILE:CD1	1:B:247:ILE:HG23	2.26	0.66
1:A:283:ASP:OD2	1:A:293:LYS:HB3	1.95	0.66
1:A:211:MET:HA	1:A:214:ARG:NH1	2.11	0.66
1:A:145:ILE:CG2	1:A:148:PHE:HB2	2.25	0.66
1:A:129:GLU:O	1:A:133:MET:HG3	1.95	0.66
1:A:33:ARG:HB2	1:A:111:PRO:HD3	1.78	0.66
1:A:215:ASN:O	1:A:218:ARG:N	2.29	0.66
1:A:38:PHE:HB3	1:A:39:PRO:CD	2.26	0.65
1:B:129:GLU:O	1:B:133:MET:HG3	1.96	0.65
1:B:215:ASN:O	1:B:218:ARG:N	2.29	0.65
1:B:222:ALA:O	1:B:225:ASP:HB2	1.96	0.65
1:A:151:ILE:HA	1:A:154:LEU:HD12	1.76	0.65
1:A:222:ALA:O	1:A:225:ASP:HB2	1.97	0.65
1:B:38:PHE:HB3	1:B:39:PRO:HD3	1.79	0.65
1:A:286:LEU:HD12	1:A:291:ASN:HD22	1.62	0.64
1:A:57:TRP:HB2	1:A:61:GLU:OE2	1.97	0.64
1:B:14:GLU:OE1	1:B:239:ASN:HB2	1.97	0.64
1:A:38:PHE:O	1:A:40:ILE:N	2.30	0.64
1:B:38:PHE:HB3	1:B:39:PRO:CD	2.27	0.64
1:B:19:LYS:HA	1:B:22:GLU:HG3	1.80	0.64
1:B:254:GLU:HG3	1:B:278:ILE:HD13	1.77	0.64
1:B:258:TYR:HA	1:B:262:LEU:O	1.98	0.64
1:B:286:LEU:HD12	1:B:291:ASN:HD22	1.63	0.64
1:B:38:PHE:O	1:B:40:ILE:N	2.31	0.64
1:A:19:LYS:HA	1:A:22:GLU:HG3	1.80	0.63
1:B:77:ASP:O	1:B:78:GLN:C	2.37	0.63
1:B:247:ILE:O	1:B:251:VAL:HG23	1.99	0.63
1:A:84:ASN:HB3	1:A:262:LEU:HD21	1.81	0.63
1:A:247:ILE:O	1:A:251:VAL:HG23	1.99	0.62
1:A:258:TYR:HA	1:A:262:LEU:O	1.98	0.62
1:B:87:ALA:HA	1:B:90:ILE:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD11	1:B:134:MET:HG2	1.81	0.62
1:B:84:ASN:HB3	1:B:262:LEU:HD21	1.81	0.62
1:A:29:MET:HA	1:A:29:MET:CE	2.30	0.62
1:B:199:TRP:O	1:B:202:ASP:HB3	2.00	0.62
1:B:65:ALA:C	1:B:67:ASP:N	2.53	0.62
1:A:198:PHE:CD2	1:A:213:ASN:ND2	2.68	0.62
1:B:62:ILE:HD13	1:B:212:ALA:HB2	1.82	0.62
1:A:50:LYS:HD3	1:A:53:GLU:OE1	1.99	0.62
1:A:199:TRP:O	1:A:202:ASP:HB3	2.00	0.62
1:A:14:GLU:OE1	1:A:239:ASN:HB2	2.00	0.61
1:B:33:ARG:HB2	1:B:111:PRO:HD3	1.81	0.61
1:A:255:LYS:HD3	1:A:275:HIS:CE1	2.35	0.61
1:B:65:ALA:C	1:B:67:ASP:H	2.03	0.61
1:A:77:ASP:O	1:A:78:GLN:C	2.38	0.61
1:A:239:ASN:C	1:A:239:ASN:ND2	2.55	0.61
1:B:50:LYS:HD3	1:B:53:GLU:OE1	2.01	0.61
1:B:42:TYR:HB2	1:B:112:GLU:OE2	2.01	0.60
1:A:42:TYR:HB2	1:A:112:GLU:OE2	2.01	0.60
1:B:201:THR:HB	1:B:210:ALA:HB2	1.82	0.60
1:A:62:ILE:HD13	1:A:212:ALA:HB2	1.83	0.60
1:A:188:ILE:HD11	1:A:247:ILE:HG23	1.84	0.60
1:B:263:PRO:C	1:B:265:GLU:H	2.03	0.60
1:A:263:PRO:C	1:A:265:GLU:H	2.03	0.60
1:B:192:GLY:HA3	1:B:258:TYR:CZ	2.37	0.60
1:B:201:THR:HA	1:B:205:ILE:HB	1.84	0.60
1:A:285:LEU:O	1:A:289:PHE:HD1	1.85	0.60
1:B:198:PHE:CD2	1:B:213:ASN:ND2	2.70	0.60
1:B:29:MET:CE	1:B:29:MET:HA	2.32	0.59
1:A:64:LEU:HD11	1:A:134:MET:HG2	1.83	0.59
1:A:201:THR:HA	1:A:205:ILE:HB	1.84	0.59
1:A:130:VAL:O	1:A:134:MET:HG3	2.03	0.59
1:A:65:ALA:C	1:A:67:ASP:N	2.55	0.59
1:A:26:ILE:CA	1:A:29:MET:HB2	2.26	0.59
1:B:255:LYS:HD3	1:B:275:HIS:CE1	2.37	0.59
1:A:239:ASN:HD22	1:A:241:LYS:H	1.49	0.59
1:A:251:VAL:HG21	1:A:295:TYR:CE1	2.38	0.59
1:B:239:ASN:HD22	1:B:241:LYS:H	1.50	0.59
1:B:175:TYR:HD2	1:B:234:LEU:HD21	1.67	0.58
1:A:192:GLY:HA3	1:A:258:TYR:CZ	2.38	0.58
1:A:258:TYR:HB3	1:A:264:VAL:HG21	1.85	0.58
1:B:285:LEU:O	1:B:289:PHE:HD1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:HA	1:A:90:ILE:HG22	1.84	0.58
1:B:111:PRO:HG2	1:B:112:GLU:H	1.68	0.58
1:A:220:ARG:HG3	1:A:220:ARG:HH21	1.67	0.58
1:B:188:ILE:HD11	1:B:247:ILE:HG23	1.86	0.58
1:B:234:LEU:HD12	1:B:234:LEU:N	2.19	0.58
1:B:262:LEU:HD23	1:B:262:LEU:N	2.19	0.58
1:A:262:LEU:N	1:A:262:LEU:HD23	2.18	0.58
1:A:234:LEU:N	1:A:234:LEU:HD12	2.19	0.57
1:B:258:TYR:HB3	1:B:264:VAL:HG21	1.86	0.57
1:A:201:THR:HB	1:A:210:ALA:HB2	1.84	0.57
1:A:65:ALA:C	1:A:67:ASP:H	2.05	0.57
1:B:179:LEU:HD21	1:B:230:LEU:HB3	1.85	0.57
1:B:26:ILE:CA	1:B:29:MET:HB2	2.25	0.57
1:B:251:VAL:HG21	1:B:295:TYR:CE1	2.40	0.57
1:B:168:ILE:O	1:B:170:ASN:N	2.37	0.57
1:A:168:ILE:O	1:A:170:ASN:N	2.37	0.57
1:A:179:LEU:HD21	1:A:230:LEU:HB3	1.86	0.56
1:A:175:TYR:HD2	1:A:234:LEU:HD21	1.70	0.56
1:A:111:PRO:HG2	1:A:112:GLU:H	1.70	0.56
1:B:130:VAL:O	1:B:134:MET:HG3	2.05	0.56
1:A:245:LYS:HB3	1:A:245:LYS:HZ2	1.70	0.56
1:B:263:PRO:O	1:B:264:VAL:HB	2.06	0.56
1:A:134:MET:HE2	1:A:209:LEU:HD13	1.88	0.56
1:B:218:ARG:O	1:B:221:GLY:N	2.34	0.55
1:A:63:GLU:CD	1:A:63:GLU:H	2.10	0.55
1:A:62:ILE:HD12	1:A:130:VAL:CG2	2.37	0.55
1:A:62:ILE:HD12	1:A:130:VAL:HG22	1.88	0.55
1:B:220:ARG:HG3	1:B:220:ARG:HH21	1.70	0.55
1:A:167:TRP:O	1:A:178:ARG:HG2	2.07	0.55
1:A:75:THR:HG23	1:A:78:GLN:OE1	2.08	0.54
1:A:301:PHE:HB2	1:A:303:PHE:CD1	2.43	0.54
1:B:301:PHE:HB2	1:B:303:PHE:CD1	2.42	0.54
1:B:245:LYS:HB3	1:B:245:LYS:NZ	2.22	0.54
1:B:77:ASP:C	1:B:79:LYS:N	2.58	0.54
1:A:263:PRO:O	1:A:264:VAL:HB	2.06	0.54
1:A:29:MET:HA	1:A:29:MET:HE2	1.89	0.54
1:A:176:ALA:O	1:A:180:VAL:HG23	2.07	0.54
1:B:63:GLU:CD	1:B:63:GLU:H	2.10	0.54
1:A:147:LEU:CD1	1:A:154:LEU:HD11	2.24	0.54
1:A:254:GLU:HG3	1:A:278:ILE:CD1	2.38	0.53
1:B:62:ILE:HB	1:B:133:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:TRP:O	1:B:178:ARG:HG2	2.07	0.53
1:B:176:ALA:O	1:B:180:VAL:HG23	2.07	0.53
1:A:247:ILE:H	1:A:247:ILE:HD12	1.73	0.53
1:B:173:SER:OG	1:B:178:ARG:NH1	2.42	0.53
1:A:68:THR:O	1:A:71:PHE:HB3	2.09	0.53
1:B:318:LYS:O	1:B:322:ASP:OD1	2.26	0.53
1:A:189:PHE:O	1:A:190:GLN:HB2	2.08	0.53
1:A:181:ALA:O	1:A:184:ALA:HB3	2.09	0.53
1:B:192:GLY:HA3	1:B:258:TYR:OH	2.08	0.53
1:A:239:ASN:HD22	1:A:240:PRO:CD	2.21	0.53
1:A:215:ASN:O	1:A:216:ILE:C	2.46	0.53
1:A:110:ASN:HD21	1:A:112:GLU:HB2	1.72	0.53
1:A:69:GLU:O	1:A:71:PHE:N	2.42	0.53
1:B:189:PHE:O	1:B:190:GLN:HB2	2.09	0.53
1:B:247:ILE:HD12	1:B:247:ILE:H	1.73	0.53
1:A:245:LYS:HB3	1:A:245:LYS:NZ	2.24	0.53
1:A:318:LYS:O	1:A:322:ASP:OD1	2.26	0.53
1:B:239:ASN:HD22	1:B:240:PRO:CD	2.22	0.53
1:B:274:ILE:HD13	1:B:301:PHE:CZ	2.44	0.53
1:A:77:ASP:C	1:A:79:LYS:N	2.58	0.53
1:A:34:ARG:HH21	1:B:102:GLU:CD	2.12	0.53
1:B:87:ALA:HA	1:B:90:ILE:CG2	2.38	0.52
1:B:286:LEU:HD12	1:B:291:ASN:HB3	1.91	0.52
1:B:15:ARG:O	1:B:19:LYS:HE2	2.09	0.52
1:A:154:LEU:HD22	1:A:156:GLU:OE2	2.10	0.52
1:A:134:MET:CE	1:A:209:LEU:HD13	2.39	0.52
1:B:62:ILE:HD12	1:B:130:VAL:CG2	2.40	0.52
1:A:274:ILE:HD13	1:A:301:PHE:CZ	2.45	0.52
1:B:215:ASN:O	1:B:216:ILE:C	2.48	0.52
1:B:63:GLU:OE2	1:B:63:GLU:N	2.42	0.52
1:B:69:GLU:O	1:B:71:PHE:N	2.42	0.52
1:B:181:ALA:O	1:B:184:ALA:HB3	2.10	0.52
1:A:87:ALA:HA	1:A:90:ILE:CG2	2.39	0.52
1:A:255:LYS:HD3	1:A:275:HIS:ND1	2.24	0.52
1:A:279:GLU:OE1	1:A:295:TYR:HB3	2.10	0.52
1:A:62:ILE:HB	1:A:133:MET:HE1	1.92	0.52
1:B:134:MET:CE	1:B:209:LEU:HD13	2.40	0.51
1:A:63:GLU:OE2	1:A:63:GLU:N	2.42	0.51
1:A:45:ILE:HG23	1:A:226:PHE:CZ	2.45	0.51
1:B:147:LEU:CD1	1:B:154:LEU:HD11	2.24	0.51
1:A:286:LEU:HD12	1:A:291:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:O	1:A:324:GLN:HG3	2.10	0.51
1:B:254:GLU:HG3	1:B:278:ILE:CD1	2.40	0.51
1:A:113:GLY:C	1:A:115:SER:H	2.13	0.51
1:B:62:ILE:HD12	1:B:130:VAL:HG22	1.91	0.51
1:A:102:GLU:CD	1:B:34:ARG:HH21	2.14	0.51
1:B:154:LEU:HD22	1:B:156:GLU:OE2	2.10	0.51
1:B:68:THR:O	1:B:71:PHE:HB3	2.10	0.51
1:B:110:ASN:HD21	1:B:112:GLU:HB2	1.74	0.51
1:B:220:ARG:HA	1:B:223:TYR:CD1	2.46	0.51
1:A:192:GLY:HA3	1:A:258:TYR:OH	2.10	0.51
1:A:279:GLU:HB3	1:A:295:TYR:CB	2.41	0.51
1:A:321:SER:HA	1:A:324:GLN:CD	2.31	0.51
1:B:75:THR:HG23	1:B:78:GLN:OE1	2.11	0.51
1:A:11:PHE:HE2	1:A:239:ASN:OD1	1.94	0.50
1:B:279:GLU:OE1	1:B:295:TYR:HB3	2.11	0.50
1:A:245:LYS:NZ	1:A:249:GLU:HG3	2.26	0.50
1:A:198:PHE:HD1	1:A:303:PHE:CZ	2.29	0.50
1:A:173:SER:OG	1:A:178:ARG:NH1	2.43	0.50
1:B:11:PHE:HE2	1:B:239:ASN:OD1	1.93	0.50
1:B:247:ILE:HB	1:B:286:LEU:HD21	1.94	0.50
1:B:299:ASN:HD21	1:B:303:PHE:HB2	1.76	0.50
1:A:77:ASP:O	1:A:80:THR:N	2.44	0.50
1:B:29:MET:HE2	1:B:29:MET:HA	1.94	0.50
1:B:239:ASN:ND2	1:B:239:ASN:C	2.54	0.50
1:A:247:ILE:HB	1:A:286:LEU:HD21	1.94	0.50
1:B:166:ARG:NH1	1:B:249:GLU:OE2	2.43	0.50
1:B:11:PHE:CD1	1:B:11:PHE:N	2.80	0.50
1:A:45:ILE:HG23	1:A:226:PHE:HZ	1.76	0.50
1:A:220:ARG:HA	1:A:223:TYR:CD1	2.47	0.49
1:B:123:MET:O	1:B:126:ILE:N	2.45	0.49
1:A:123:MET:O	1:A:126:ILE:N	2.44	0.49
1:A:164:ILE:HD12	1:A:164:ILE:N	2.26	0.49
1:B:84:ASN:CB	1:B:262:LEU:HD21	2.42	0.49
1:B:247:ILE:HD12	1:B:247:ILE:N	2.27	0.49
1:A:299:ASN:HD21	1:A:303:PHE:HB2	1.76	0.49
1:B:321:SER:HA	1:B:324:GLN:CD	2.33	0.49
1:B:77:ASP:O	1:B:80:THR:N	2.45	0.49
1:A:15:ARG:O	1:A:19:LYS:HE2	2.12	0.49
1:A:65:ALA:O	1:A:66:LYS:HB2	2.12	0.49
1:A:35:PHE:HE1	1:B:99:TYR:CD1	2.31	0.49
1:B:279:GLU:HB3	1:B:295:TYR:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HD12	1:A:27:LEU:N	2.28	0.49
1:A:247:ILE:HD12	1:A:247:ILE:N	2.28	0.49
1:A:244:GLU:O	1:A:245:LYS:C	2.50	0.49
1:A:146:PRO:O	1:A:148:PHE:N	2.45	0.49
1:B:33:ARG:NH1	1:B:33:ARG:HG2	2.28	0.49
1:B:45:ILE:HG23	1:B:226:PHE:CZ	2.47	0.49
1:A:194:TYR:OH	1:A:220:ARG:HD2	2.13	0.49
1:B:255:LYS:HD3	1:B:275:HIS:ND1	2.26	0.49
1:A:166:ARG:NH1	1:A:249:GLU:OE2	2.44	0.49
1:B:27:LEU:HD21	1:B:230:LEU:CD2	2.43	0.48
1:A:11:PHE:N	1:A:11:PHE:CD1	2.81	0.48
1:B:261:SER:C	1:B:262:LEU:HD23	2.33	0.48
1:A:84:ASN:CB	1:A:262:LEU:HD21	2.43	0.48
1:A:321:SER:HA	1:A:324:GLN:OE1	2.12	0.48
1:A:130:VAL:O	1:A:133:MET:HB2	2.13	0.48
1:A:154:LEU:HB2	1:A:157:VAL:HG13	1.94	0.48
1:B:146:PRO:O	1:B:148:PHE:N	2.46	0.48
1:A:86:LEU:O	1:A:90:ILE:HG22	2.13	0.48
1:A:26:ILE:HD12	1:A:26:ILE:C	2.33	0.48
1:B:26:ILE:HD12	1:B:27:LEU:N	2.29	0.48
1:A:261:SER:C	1:A:262:LEU:HD23	2.34	0.48
1:B:320:VAL:O	1:B:324:GLN:HG3	2.12	0.48
1:A:70:ASP:HB2	1:A:206:MET:HG3	1.95	0.48
1:A:139:PHE:O	1:A:141:ASP:N	2.41	0.48
1:B:164:ILE:HD12	1:B:164:ILE:N	2.28	0.48
1:B:321:SER:HA	1:B:324:GLN:OE1	2.14	0.48
1:B:198:PHE:HD1	1:B:303:PHE:CZ	2.31	0.48
1:B:162:ALA:O	1:B:166:ARG:HB2	2.14	0.48
1:B:141:ASP:CG	1:B:142:PRO:HD2	2.34	0.48
1:A:160:LYS:HZ1	1:A:189:PHE:HB3	1.78	0.48
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.29	0.48
1:B:244:GLU:O	1:B:245:LYS:C	2.53	0.48
1:B:130:VAL:O	1:B:133:MET:HB2	2.12	0.48
1:B:70:ASP:HB2	1:B:206:MET:HG3	1.96	0.48
1:A:270:ASP:O	1:A:272:LYS:N	2.47	0.48
1:A:176:ALA:HB2	1:A:234:LEU:HD22	1.94	0.48
1:A:186:GLU:OE2	1:A:220:ARG:HG2	2.14	0.48
1:B:186:GLU:OE2	1:B:220:ARG:HG2	2.14	0.48
1:B:245:LYS:NZ	1:B:249:GLU:HG3	2.29	0.48
1:A:27:LEU:HD21	1:A:230:LEU:CD2	2.43	0.48
1:A:220:ARG:NH2	1:A:220:ARG:HG3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:C	1:B:115:SER:H	2.16	0.47
1:B:238:PRO:O	1:B:239:ASN:C	2.53	0.47
1:B:199:TRP:O	1:B:200:LEU:O	2.32	0.47
1:B:139:PHE:O	1:B:141:ASP:N	2.43	0.47
1:B:26:ILE:C	1:B:26:ILE:HD12	2.35	0.47
1:B:202:ASP:O	1:B:203:LYS:HB2	2.13	0.47
1:B:60:GLU:N	1:B:60:GLU:OE2	2.47	0.47
1:A:200:LEU:O	1:A:202:ASP:N	2.48	0.47
1:A:99:TYR:CD1	1:B:35:PHE:HE1	2.32	0.47
1:B:200:LEU:O	1:B:205:ILE:HD12	2.13	0.47
1:B:45:ILE:HG23	1:B:226:PHE:HZ	1.79	0.47
1:B:215:ASN:O	1:B:218:ARG:HB3	2.15	0.47
1:B:57:TRP:HB2	1:B:61:GLU:CD	2.35	0.47
1:A:131:TYR:C	1:A:133:MET:H	2.18	0.47
1:A:62:ILE:CD1	1:A:212:ALA:HB2	2.43	0.47
1:B:134:MET:HE2	1:B:209:LEU:HD13	1.95	0.47
1:B:62:ILE:CD1	1:B:212:ALA:HB2	2.43	0.47
1:A:162:ALA:O	1:A:166:ARG:HB2	2.14	0.47
1:B:63:GLU:O	1:B:63:GLU:HG2	2.15	0.47
1:A:141:ASP:CG	1:A:142:PRO:HD2	2.35	0.47
1:B:160:LYS:HZ1	1:B:189:PHE:HB3	1.79	0.47
1:A:180:VAL:O	1:A:183:ALA:HB3	2.14	0.47
1:A:168:ILE:HG22	1:A:169:SER:N	2.29	0.47
1:A:60:GLU:N	1:A:60:GLU:OE2	2.48	0.47
1:B:154:LEU:HB2	1:B:157:VAL:HG13	1.96	0.46
1:A:200:LEU:O	1:A:205:ILE:HD12	2.15	0.46
1:B:200:LEU:O	1:B:202:ASP:N	2.48	0.46
1:B:176:ALA:HB2	1:B:234:LEU:HD22	1.97	0.46
1:A:57:TRP:HB2	1:A:61:GLU:CD	2.35	0.46
1:B:270:ASP:O	1:B:272:LYS:N	2.48	0.46
1:A:238:PRO:O	1:A:239:ASN:C	2.52	0.46
1:B:33:ARG:HH11	1:B:33:ARG:HG2	1.80	0.46
1:B:194:TYR:OH	1:B:220:ARG:HD2	2.16	0.46
1:B:65:ALA:O	1:B:66:LYS:HB2	2.14	0.46
1:A:239:ASN:ND2	1:A:240:PRO:HD2	2.31	0.46
1:A:262:LEU:HA	1:A:263:PRO:HD3	1.75	0.46
1:B:31:ASN:ND2	1:B:32:SER:H	2.13	0.46
1:A:199:TRP:O	1:A:200:LEU:O	2.33	0.46
1:A:202:ASP:O	1:A:203:LYS:HB2	2.16	0.46
1:B:86:LEU:O	1:B:90:ILE:HG22	2.15	0.46
1:B:168:ILE:HG22	1:B:169:SER:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:HA	1:A:142:PRO:HD3	1.85	0.46
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.81	0.46
1:A:63:GLU:O	1:A:63:GLU:HG2	2.16	0.46
1:B:220:ARG:NH2	1:B:220:ARG:HG3	2.31	0.46
1:A:64:LEU:HD13	1:A:137:ALA:CB	2.46	0.46
1:B:239:ASN:ND2	1:B:240:PRO:HD2	2.32	0.45
1:A:31:ASN:ND2	1:A:32:SER:H	2.14	0.45
1:A:71:PHE:CE2	1:A:138:PHE:HB2	2.51	0.45
1:B:71:PHE:CE2	1:B:138:PHE:HB2	2.51	0.45
1:B:82:ILE:O	1:B:85:LEU:HB3	2.17	0.45
1:A:215:ASN:O	1:A:218:ARG:HB3	2.17	0.45
1:B:64:LEU:HD13	1:B:137:ALA:CB	2.46	0.45
1:A:82:ILE:O	1:A:85:LEU:HB3	2.17	0.45
1:A:88:LEU:HD12	1:A:262:LEU:HD11	1.98	0.45
1:B:175:TYR:CD2	1:B:234:LEU:HD21	2.50	0.45
1:B:71:PHE:CD2	1:B:138:PHE:HB2	2.52	0.45
1:A:5:ASN:O	1:A:9:LYS:N	2.50	0.45
1:A:71:PHE:CD2	1:A:138:PHE:HB2	2.52	0.45
1:A:113:GLY:C	1:A:115:SER:N	2.70	0.44
1:B:131:TYR:C	1:B:133:MET:H	2.19	0.44
1:A:173:SER:CB	1:A:178:ARG:HH11	2.31	0.44
1:A:35:PHE:HE1	1:B:99:TYR:CE1	2.35	0.44
1:B:173:SER:CB	1:B:178:ARG:HH11	2.29	0.44
1:B:195:ALA:HA	1:B:303:PHE:CZ	2.39	0.44
1:A:160:LYS:HE3	1:A:160:LYS:HB2	1.88	0.44
1:B:174:LEU:O	1:B:177:GLU:HB2	2.18	0.44
1:B:240:PRO:HA	1:B:243:ILE:HG13	1.98	0.44
1:A:242:ILE:O	1:A:246:ILE:HG13	2.17	0.44
1:A:36:VAL:HG22	1:A:112:GLU:N	2.32	0.44
1:A:99:TYR:CE1	1:B:35:PHE:HE1	2.36	0.44
1:B:247:ILE:CG2	1:B:282:ALA:HB1	2.47	0.44
1:A:166:ARG:HH11	1:A:249:GLU:CD	2.20	0.44
1:A:44:GLU:O	1:A:47:ALA:N	2.51	0.44
1:A:181:ALA:O	1:A:184:ALA:N	2.51	0.44
1:A:216:ILE:HG23	1:A:220:ARG:HH21	1.82	0.43
1:B:234:LEU:CD1	1:B:234:LEU:H	2.28	0.43
1:A:247:ILE:CG2	1:A:282:ALA:HB1	2.47	0.43
1:B:96:VAL:O	1:B:100:LEU:HG	2.18	0.43
1:B:25:GLU:OE2	1:B:234:LEU:HA	2.19	0.43
1:B:242:ILE:O	1:B:246:ILE:HG13	2.18	0.43
1:A:263:PRO:C	1:A:265:GLU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:PRO:HA	1:A:243:ILE:HG13	2.00	0.43
1:A:274:ILE:HD13	1:A:301:PHE:HZ	1.82	0.43
1:B:113:GLY:C	1:B:115:SER:N	2.72	0.43
1:B:36:VAL:HG22	1:B:112:GLU:N	2.33	0.43
1:B:5:ASN:O	1:B:9:LYS:N	2.51	0.43
1:A:195:ALA:HA	1:A:303:PHE:CZ	2.38	0.43
1:B:276:THR:O	1:B:279:GLU:HB2	2.18	0.43
1:A:160:LYS:O	1:A:163:PHE:HB3	2.19	0.43
1:A:198:PHE:O	1:A:199:TRP:C	2.57	0.43
1:B:180:VAL:O	1:B:183:ALA:HB3	2.17	0.43
1:B:277:TYR:O	1:B:280:PHE:HB3	2.19	0.43
1:B:160:LYS:O	1:B:163:PHE:HB3	2.18	0.43
1:A:192:GLY:O	1:A:193:ASN:C	2.57	0.43
1:A:27:LEU:HD21	1:A:230:LEU:HD22	2.00	0.43
1:A:299:ASN:HA	1:A:300:PRO:HD3	1.86	0.42
1:A:174:LEU:O	1:A:177:GLU:HB2	2.19	0.42
1:A:105:SER:HA	1:A:117:TYR:CD2	2.54	0.42
1:B:286:LEU:CD1	1:B:291:ASN:HD22	2.31	0.42
1:B:86:LEU:HD13	1:B:134:MET:HB2	2.02	0.42
1:B:181:ALA:O	1:B:184:ALA:N	2.52	0.42
1:A:96:VAL:O	1:A:100:LEU:HG	2.19	0.42
1:A:154:LEU:CB	1:A:157:VAL:HG13	2.50	0.42
1:B:88:LEU:HD12	1:B:262:LEU:HD11	2.00	0.42
1:B:263:PRO:HB3	1:B:266:LYS:HB2	2.01	0.42
1:A:157:VAL:CG2	1:A:158:LYS:N	2.82	0.42
1:B:157:VAL:CG2	1:B:158:LYS:N	2.83	0.42
1:B:160:LYS:HB2	1:B:160:LYS:HE3	1.87	0.42
1:B:315:PHE:CD2	1:B:316:PHE:N	2.88	0.42
1:B:198:PHE:O	1:B:199:TRP:C	2.57	0.42
1:B:247:ILE:HG21	1:B:286:LEU:CD2	2.50	0.42
1:B:105:SER:HA	1:B:117:TYR:CD2	2.54	0.42
1:B:157:VAL:O	1:B:160:LYS:HB3	2.20	0.42
1:B:160:LYS:O	1:B:163:PHE:N	2.52	0.42
1:A:263:PRO:HB3	1:A:266:LYS:HB2	2.01	0.42
1:B:11:PHE:C	1:B:13:LYS:H	2.23	0.42
1:B:192:GLY:O	1:B:193:ASN:C	2.57	0.42
1:B:274:ILE:HD13	1:B:301:PHE:HZ	1.82	0.42
1:A:175:TYR:CD2	1:A:234:LEU:HD21	2.53	0.42
1:B:87:ALA:C	1:B:89:SER:N	2.73	0.42
1:B:44:GLU:O	1:B:47:ALA:N	2.53	0.42
1:B:154:LEU:CB	1:B:157:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ASN:CB	1:B:262:LEU:CD2	2.98	0.41
1:A:276:THR:O	1:A:279:GLU:HB2	2.20	0.41
1:A:218:ARG:O	1:A:221:GLY:N	2.38	0.41
1:A:86:LEU:HD13	1:A:134:MET:HB2	2.02	0.41
1:B:89:SER:O	1:B:91:SER:N	2.53	0.41
1:B:229:LEU:O	1:B:233:HIS:CE1	2.73	0.41
1:B:166:ARG:HH11	1:B:249:GLU:CD	2.21	0.41
1:A:71:PHE:C	1:A:73:LYS:H	2.23	0.41
1:B:104:PHE:CZ	1:B:182:PHE:HB2	2.55	0.41
1:B:69:GLU:C	1:B:71:PHE:N	2.73	0.41
1:A:286:LEU:CD1	1:A:291:ASN:HD22	2.30	0.41
1:A:240:PRO:HB3	1:A:291:ASN:OD1	2.20	0.41
1:B:78:GLN:HA	1:B:267:PHE:HD1	1.86	0.41
1:A:84:ASN:OD1	1:A:147:LEU:HB2	2.21	0.41
1:A:11:PHE:C	1:A:13:LYS:H	2.23	0.41
1:A:279:GLU:HB2	1:A:297:ALA:HB2	2.03	0.41
1:A:69:GLU:C	1:A:71:PHE:N	2.73	0.41
1:B:27:LEU:HD21	1:B:230:LEU:HD22	2.01	0.41
1:B:240:PRO:HB3	1:B:291:ASN:OD1	2.21	0.41
1:B:210:ALA:O	1:B:214:ARG:HB2	2.20	0.41
1:A:160:LYS:O	1:A:163:PHE:N	2.54	0.41
1:A:277:TYR:O	1:A:278:ILE:C	2.59	0.41
1:A:277:TYR:O	1:A:280:PHE:HB3	2.20	0.41
1:B:188:ILE:HD13	1:B:247:ILE:HG23	2.01	0.41
1:A:315:PHE:CD2	1:A:316:PHE:N	2.88	0.41
1:A:234:LEU:CD1	1:A:234:LEU:H	2.29	0.41
1:A:25:GLU:OE2	1:A:234:LEU:HA	2.21	0.41
1:A:225:ASP:O	1:A:228:CYS:HB2	2.21	0.41
1:B:141:ASP:HA	1:B:142:PRO:HD3	1.86	0.41
1:B:122:MET:HB3	1:B:122:MET:HE2	1.96	0.41
1:A:255:LYS:O	1:A:257:TYR:N	2.54	0.41
1:A:94:ASN:O	1:A:98:LYS:HG3	2.21	0.41
1:B:284:GLY:HA2	1:B:287:GLN:OE1	2.20	0.41
1:B:84:ASN:OD1	1:B:147:LEU:HB2	2.21	0.40
1:A:13:LYS:HD2	1:A:13:LYS:N	2.36	0.40
1:A:210:ALA:O	1:A:214:ARG:HB2	2.21	0.40
1:A:38:PHE:CB	1:A:39:PRO:CD	2.97	0.40
1:A:104:PHE:CZ	1:A:182:PHE:HB2	2.56	0.40
1:A:30:GLU:N	1:A:109:GLN:HG3	2.36	0.40
1:A:239:ASN:ND2	1:A:240:PRO:CD	2.84	0.40
1:B:38:PHE:CB	1:B:39:PRO:CD	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ALA:C	1:B:89:SER:H	2.23	0.40
1:B:277:TYR:O	1:B:278:ILE:C	2.59	0.40
1:B:255:LYS:O	1:B:257:TYR:N	2.55	0.40
1:A:247:ILE:HG21	1:A:286:LEU:CD2	2.51	0.40
1:A:170:ASN:OD1	1:A:172:ASP:N	2.55	0.40
1:B:207:PRO:O	1:B:208:GLY:C	2.59	0.40
1:A:284:GLY:HA2	1:A:287:GLN:OE1	2.22	0.40
1:B:71:PHE:C	1:B:73:LYS:H	2.25	0.40
1:A:229:LEU:O	1:A:233:HIS:CE1	2.75	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	310/345 (90%)	225 (73%)	51 (16%)	34 (11%)	0 3
1	B	310/345 (90%)	224 (72%)	52 (17%)	34 (11%)	0 3
All	All	620/690 (90%)	449 (72%)	103 (17%)	68 (11%)	0 3

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	38	PHE
1	A	39	PRO
1	A	200	LEU
1	A	263	PRO
1	A	264	VAL
1	A	271	LEU
1	B	33	ARG
1	B	38	PHE

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Mol	Chain	Res	Type
1	B	39	PRO
1	B	200	LEU
1	B	263	PRO
1	B	264	VAL
1	B	271	LEU
1	A	36	VAL
1	A	70	ASP
1	A	90	ILE
1	A	140	LYS
1	A	146	PRO
1	A	147	LEU
1	A	149	LYS
1	A	169	SER
1	A	201	THR
1	A	216	ILE
1	A	256	GLU
1	A	261	SER
1	B	36	VAL
1	B	70	ASP
1	B	90	ILE
1	B	146	PRO
1	B	147	LEU
1	B	149	LYS
1	B	169	SER
1	B	201	THR
1	B	216	ILE
1	B	256	GLU
1	B	261	SER
1	A	12	GLN
1	A	69	GLU
1	A	75	THR
1	A	196	SER
1	A	203	LYS
1	A	215	ASN
1	B	12	GLN
1	B	69	GLU
1	B	75	THR
1	B	140	LYS
1	B	196	SER
1	B	203	LYS
1	B	215	ASN
1	B	218	ARG

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Mol	Chain	Res	Type
1	A	302	GLU
1	B	144	ASN
1	B	302	GLU
1	A	30	GLU
1	A	65	ALA
1	A	144	ASN
1	A	218	ARG
1	A	288	GLY
1	B	30	GLU
1	B	65	ALA
1	B	288	GLY
1	A	72	GLN
1	A	206	MET
1	B	206	MET
1	A	168	ILE
1	B	111	PRO
1	B	168	ILE

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	276/303 (91%)	248 (90%)	28 (10%)	9 33
1	B	276/303 (91%)	250 (91%)	26 (9%)	11 39
All	All	552/606 (91%)	498 (90%)	54 (10%)	10 36

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	20	GLU
1	A	25	GLU
1	A	29	MET
1	A	33	ARG
1	A	38	PHE

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Mol	Chain	Res	Type
1	A	39	PRO
1	A	44	GLU
1	A	63	GLU
1	A	70	ASP
1	A	110	ASN
1	A	114	LYS
1	A	121	ILE
1	A	138	PHE
1	A	148	PHE
1	A	156	GLU
1	A	157	VAL
1	A	198	PHE
1	A	236	THR
1	A	239	ASN
1	A	241	LYS
1	A	263	PRO
1	A	269	MET
1	A	275	HIS
1	A	283	ASP
1	A	286	LEU
1	A	301	PHE
1	A	304	MET
1	B	16	HIS
1	B	20	GLU
1	B	25	GLU
1	B	29	MET
1	B	33	ARG
1	B	38	PHE
1	B	39	PRO
1	B	63	GLU
1	B	70	ASP
1	B	110	ASN
1	B	114	LYS
1	B	121	ILE
1	B	138	PHE
1	B	148	PHE
1	B	157	VAL
1	B	198	PHE
1	B	236	THR
1	B	239	ASN
1	B	241	LYS
1	B	263	PRO

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Mol	Chain	Res	Type
1	B	269	MET
1	B	275	HIS
1	B	283	ASP
1	B	286	LEU
1	B	301	PHE
1	B	304	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	31	ASN
1	A	72	GLN
1	A	110	ASN
1	A	120	GLN
1	A	190	GLN
1	A	239	ASN
1	B	6	GLN
1	B	31	ASN
1	B	72	GLN
1	B	110	ASN
1	B	120	GLN
1	B	190	GLN
1	B	239	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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